

Boltzmannian Framework for Macroscopic Quantum Systems

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Zusammenfassung

In dieser Arbeit beschreiben wir das boltzmannsche Paradigma als einen grundlegenden Rahmen für die quantenstatistische Mechanik geschlossener makroskopischer Systeme. Wir formulieren neue Vorschläge für den zweiten Hauptsatz der Thermodynamik, verifizieren ihn für einfache zufällige Hamiltonoperatoren und begründen die Verwendung thermodynamischer Ensembles, wobei wir insbesondere die Grundlagen des großkanonischen Ensembles erläutern.

Der erste Teil der Arbeit führt das boltzmannsche Paradigma als einen kohärenten konzeptuellen Rahmen ein, das thermische Verhalten eines geschlossenen makroskopischen Quantensystems $\mathcal{S}$ zu beschreiben. Für solche Systeme mit einem D -dimensionalen Hilbertraum $\mathcal{H}$ wird der Mikrozustand durch eine Wellenfunktion $\psi \in \mathcal{H}$ gegeben, die sich unitär entwickelt gemäß $\psi_t = e^{-iHt}\psi_0$. In Anlehnung an von Neumann zerlegen wir $\mathcal{H}$ in orthogonale Unterräume $\mathcal{H}_\nu$, wobei jedes ν als ein Makrozustand ν verstanden wird; verschiedene Wellenfunktionen $\psi, \phi \in \mathcal{H}_\nu$ repräsentieren denselben Makrozustand ν . Unter diesen Unterräumen befindet sich ein Unterraum $\mathcal{H}_{\text{eq}}$, der bei weitem den überwiegenden Anteil der Dimensionen besitzt, $d_{\text{eq}}/D \approx 1$, sodass jedes ψ , das beliebig nahe an $\mathcal{H}_{\text{eq}}$ liegt, ein makroskopisches thermisches Equilibrium (MATE) repräsentiert. Die Annäherung an MATE bedeutet, dass die unitäre Zeitentwicklung eines Anfangszustands ψ_0 so verläuft, dass ψ_t die meiste Zeit nahe bei $\mathcal{H}_{\text{eq}}$ liegt. Diese Annäherung ist universell in dem Sinne, dass sich die meisten Anfangswellenfunktionen in MATE entwickeln. Wir heben außerdem die Bedeutung der Argumentationsweise Boltzmanns in der Physik hervor.

Im zweiten Teil diskutieren wir den Status des zweiten Hauptsatzes in makroskopischen Quantensystemen. Zunächst argumentieren wir, dass die quantenmechanische Boltzmann-Entropie $S_{\text{QB}}(\nu) = k_B \log \dim \mathcal{H}_\nu$ diejenige Größe ist, die für das Verständnis des zweiten Hauptsatzes relevant ist. Anschließend präsentieren wir zwei neue Vorschläge dafür, was es bedeutet, dass $S_{\text{QB}}(\nu)$ mit der Zeit wächst. Beide beruhen auf der Idee, dass die Entropie zunimmt, wenn Wahrscheinlichkeit in Unterräume mit größerer Dimension transportiert wird. Die Zeitentwicklung eines Makrozustands ν , gegeben durch $\|\hat{P}_\nu \psi_t\|^2$, wobei $\hat{P}_\nu$ der Projektor auf $\mathcal{H}_\nu$ ist, liefert für jedes t eine Verteilung auf der (geordneten) Menge der Makrozustände. Wir schlagen vor, dass sich eine solche Verteilung typischerweise nach rechts bewegt, das heißt, dass größere Entropiewerte größere Gewichte erhalten und daher die Entropie zunimmt. Ein weiterer Vorschlag erfolgt über einen Wahrscheinlichkeitsstrom $J_{\nu\nu'}(t)$, der von ν' nach ν fließt. Wenn Wahrscheinlichkeit überwiegend in größere Unter-

räume fließt, ist auch dies ein Ausdruck eines Entropieanstiegs. Diese Versionen werden durch ein Zufallsmatrixmodell validiert. Darüber hinaus schlagen wir einen allgemeinen Ansatz vor, um $||\hat{P}_\nu\psi_t||^2$ und $J_{\nu\nu'}(t)$ zu berechnen.

Im dritten Teil diskutieren wir die Rechtfertigung thermodynamischer Ensembles und konzentrieren uns insbesondere auf das großkanonische Ensemble. Wir erörtern, wie reine Zustände das thermische Equilibrium kleiner Teilsysteme beschreiben können. Außerdem stellen wir neue Einsichten darüber vor, wie das großkanonische Ensemble aus chemischen Reaktionen hervorgeht. Darüber hinaus führen wir neue Resultate für Systeme mit mehreren Erhaltungsgrößen, reduzierte Dichtematrizen sowie Wellenfunktionen mit typischem Verhalten ein. Diese unterscheiden sich von den bisherigen GAP-Maßen insofern, als sie Summen von GAP-Maßen darstellen. Wir erweitern außerdem Resultate über GAP-Maße, die als Equilibriumsverteilungen für Wellenfunktionen von Teilsystemen dienen und als quantenmechanische Analoga klassischer thermodynamischer Ensembles betrachtet werden können. Jeder Dichtematrix $\hat{\rho}$ kann man ein Maß $\text{GAP}_{\hat{\rho}}$ zuordnen, sodass man insbesondere für kanonischen Dichtematrizen $\text{GAP}_{\hat{\rho}}$ als eine universelle und natürliche Verteilung für Wellenfunktionen erhält. Anschließend diskutieren wir, wie ein reiner Zustand Ψ eines geschlossenen Systems für geeignete Observablen dieselbe Born-Verteilung liefern kann wie die kanonische Dichtematrix $\hat{\rho}_{\text{can}}$ auf einem Teilsystem. Da dies für die meisten solchen Wellenfunktionen der Fall ist, argumentieren wir, dass Ensembles typisch sind. Wir kontrastieren diese Sichtweise mit anderen Auffassungen in der Literatur, insbesondere mit “subjektiven” Ansätzen wie dem Maximum-Entropie-Prinzip. Unsere Auffassung ist, dass thermisches Equilibrium das typische Verhalten darstellt: So verhalten sich die meisten Mikrozustände, und dies zeigt, wie Ensembles sowie thermische Verteilungen von Wellenfunktionen in der Natur auftreten.

Summary

In this thesis we describe the Boltzmannian quantum framework (BQF) as a fundamental framework for quantum statistical mechanics (QSM) of closed macroscopic systems. We state novel proposals for the second law of thermodynamics, verifying it for simple random Hamiltonians and justify the use of thermodynamic ensembles, in particular explaining foundations of the grand-canonical ensemble.

The first part of the thesis introduces the BQF as a coherent way to describe thermal behavior of a closed macroscopic quantum system $\mathcal{S}$, in particular thermalization. For such systems, with D -dimensional Hilbert space $\mathcal{H}$, the micro state is given by a wave function $\psi \in \mathcal{H}$, evolving unitarily $\psi_t = e^{-iHt}\psi_0$. Following von Neumann we decompose $\mathcal{H}$ into orthogonal subspaces $\mathcal{H}_\nu$, for which each ν is understood as a macro state ν ; different wave functions $\psi, \phi \in \mathcal{H}_\nu$ represent the same macrostate ν . Among these subspaces is a subspace $\mathcal{H}_{\text{eq}}$, which has by far the overwhelming majority of dimensions $d_{\text{eq}}/D \approx 1$, such that any ψ being arbitrarily close to $\mathcal{H}_{\text{eq}}$ represents macroscopic thermal equilibrium (MATE). The approach to MATE means that the unitary evolution of an initial state ψ_0 is such that ψ_t will be close to $\mathcal{H}_{\text{eq}}$ most of the time. This approach is universal, in the sense that most initial wave functions will evolve into MATE. We also highlight the importance of Boltzmann's reasoning in physics.

In the second part we discuss the status of the second law in macroscopic quantum systems. First arguing that the quantum Boltzmann entropy $S_{\text{QB}}(\nu) = k_B \log \dim \mathcal{H}_\nu$ is the one relevant for understanding the second law. Then we present two novel proposals for what it means that $S_{\text{QB}}(\nu)$ increases with time. Both of them build on the idea that if probability is transported to subspaces with larger dimension, then entropy increases. The time evolution of a macro state ν is given by $\|\hat{P}_\nu \psi_t\|^2$, where $\hat{P}_\nu$ is the projector onto $\mathcal{H}_\nu$, yields for each t a distribution on the (ordered) set of macro states. We propose that typically such a distribution moves to the right, that is larger entropy values get larger weights, and therefore entropy increases. Another proposal is via a probability current $J_{\nu\nu'}(t)$ flowing from ν' to ν . If probability mostly flows to larger subspaces, this is also an expression of entropy increase. These versions are validated by a random matrix model. We further propose a general ansatz to compute $\|\hat{P}_\nu \psi_t\|^2$ and $J_{\nu\nu'}(t)$.

In the third part we discuss the justification of thermodynamic ensembles and focus in particular on the grand-canonical ensemble. We discuss how pure states can describe thermal equilibrium of small subsystems. We further state novel insights on

0. Summary

how grand-canonical ensemble appears from chemical reactions. We also introduce new results for systems with multiple conserved quantities, reduced density matrices, as well as wave functions having typical behavior. These are different from the GAP measures so far as they are sums of GAP measures. We extend on results about GAP measures, which serve as thermal equilibrium distributions for wave functions of subsystems and can be viewed as quantum analogs of classical thermodynamic ensembles. To each density matrix $\hat{\rho}$ one can associate a measure $\text{GAP}_{\hat{\rho}}$, that is in particular for the canonical density matrices one obtains $\text{GAP}_{\hat{\rho}}$ as a universal and natural distribution for wave functions. Then we discuss how a pure state Ψ of a closed system can yield the same Born distribution for suitable observables as the canonical density matrix $\hat{\rho}_{\text{can}}$ on a subsystem. As this is the case for most such wave functions, we argue that ensembles are typical. We contrast this with other views in literature, especially with “subjective” views, such as the maximum entropy principle. Our view is that thermal equilibrium is the typical behavior, its how most micro states behave and that shows how ensembles as well as thermal distributions of wave functions appear in nature.

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Personal Contribution

In all articles, the authors are ordered alphabetically.

a) Submitted Manuscripts

1. Grand-Canonical Typicality

Cedric Igelspacher, Roderich Tumulka, Cornelia Vogel.

arXiv:2601.03253v2.

Included in Appendix 11.2.

Scientific Ideas: 33%. Analysis/Interpretation: 33%. Paper Writing: 33%.

List of Abbreviations

ARMD	Approximately right moving distribution
BEOM	Bohm's equation of motion
BF	Boltzmannian framework
BM	Bohmian mechanics
BQF	Boltzmannian quantum framework
BSL	Bell second law
GNE	Generalized normal equilibrium
GOE	Gaussian orthogonal ensemble
GSE	Gaussian symplectic ensemble
GUE	Gaussian unitary ensemble
MATE	Macroscopic thermal equilibrium
MEP	Maximum entropy principle
MITE	Microscopic thermal equilibrium
NE	Normal equilibrium
ODE	Ordinary differential equation
OQM	Orthodox quantum mechanics
PEP	Principle of equal a priori probabilities
PH	Past hypothesis
PO	Primitive ontology
POVM	Positive operator valued measure
QET	Quantum ergodic theorem
QSM	Quantum statistical mechanics
RMD	Right moving distribution
RPT	Rationality Principle of Typicality
VDE	Vector-Dyson-equation
WLLN	Weak law of large numbers
WSL	Weak second law
w.v.h.p.	with very high probability

Quotes

“Mit der Idee der atomistischen Weltbeschreibung der Vorsokratiker kommt gleichzeitig eine Weltordnung, ein durch ein Weltgesetz geregelter Ablauf im Kosmos.”[80, p.2]

“Incidentally, he [Res Jost, C.I.] also warned some of us that, at a party, one should never start a conversation about:

- irreversibility and the arrow of time;
- the foundations and the “interpretation” of Quantum Mechanics;
- religious faith.

”[106, p.3]

a bird is a bird,
slavery means slavery,
a knife is a knife,
death remains death.

– Zbigniew Herbert¹

“Und noch etwas: Wenn in einer Druckerei nach einer Explosion Tausende von Bleilettern durch die Luft wirbeln, werden sie sich im Fallen wohl kaum zu einem Buch zusammensetzen. Warum? Weil Ordnung eben nie die Frucht von Zufall ist. Das hatte Motti eingeleuchtet, es hatte ihm so sehr eingeleuchtet, daß er keine Sekunde darüber nachdachte.”[20, p. 119]

“Im Handumdrehen also wird der Erzähler mit Hansens Geschichte nicht fertig werden. Die sieben Tage einer Woche werden dazu nicht reichen und auch sieben Monate nicht. Am besten ist es, er macht sich im voraus nicht klar, wieviel Erdenzeit ihm verstreichen wird, während sie ihn umspinnen hält. Es werden, in Gottes Namen, ja nicht geradezu sieben Jahre sein! Und somit fangen wir an.”[191]

¹Cited from [3].

Overview

We begin with a short overview of the thesis. Let us start with an example. Think of a box divided into two parts by some constraint not interacting with the environment. One part, say the left part of the box, contains a gas, while the right part contains no gas (e.g. a vacuum). This is done by some fitting preparation procedure. After removing the constraint the gas will slowly spread out from the left half towards the right half of the box. After some time the gas particles will uniformly distribute over the whole box.

This empirically robust phenomena contains two central aspects of statistical mechanics, namely thermal equilibrium and the approach towards it [39]. It further shows a key fact, namely that the approach to thermal equilibrium is irreversible. This behavior is universal, in the sense that it does not rely on specific microscopic details of the system. Both show itself in the basic formalism of thermodynamics, which is formulated solely in terms of macroscopic variables. Concerning the approach to thermal equilibrium and the fact that its irreversible is stated in the minus first and second law of thermodynamics.

Now consider the same box and focus on a small spatial region within it as the subsystem, while the rest of the box acts as a heat bath that is sufficiently large so that its temperature does not change through interaction with the subsystem. A natural question to ask now is: how is thermal equilibrium properly described for the subsystem? What does it mean for the subsystem to be in thermal equilibrium?

The issues just stated briefly are addressed in this thesis:

1. **Problem of irreversibility:** How can entropy increase in closed macroscopic quantum systems be understood? Why do systems show macroscopic irreversible behavior, while the underlying microscopic dynamics is reversible? In other words: why do systems evolve into equilibrium?
2. **Justifying ensembles:** What justifies the use of thermodynamic ensembles? Why is a subsystem in thermal equilibrium?

It will be a main point of this thesis that both of these questions have to be looked at from the right direction. That is we also have to ask the following:

3. **Conceptual Framework:** What is a coherent framework addressing the foundations of quantum statistical mechanics properly?

As we will see the trivial fact that asking different questions will yield different answers has severe consequences with respect to the above stated issues.

The way we formulated our questions above clearly asks for the reasons and the meaning why thermal behavior appears. That is we aim for explanations of physically observed phenomena. We will see and that is what we argue below the short answer to why systems evolve to thermal equilibrium or why thermodynamic ensembles describe subsystems is because that is **typical**. In other words, it is a universal behavior, that is instantiated by most micro states. The exceptions that such a behavior does not take place are unimaginably small.

Appealing to typicality to explain irreversibility has been introduced by Ludwig Boltzmann [28]. The conceptual framework we follow is in his spirit. It relies on a clear view of what a theory fundamentally is about. It connects the microscopic with the macroscopic realm. And finally it allows to explain macroscopic (large number of degrees of freedom) emergent behavior as the typical behavior, the behavior that appears in most cases². Further this reasoning relies on a realistic or objective view, that nature does what it does independent of human beings (a view also shared by Einstein and Schrödinger [242]). In particular the behavior of microscopic systems does not rely on measurement or any knowledge that an observer might have (or not have).

We will now give an overview of the main results of this thesis.

Individualism vs. Ensemblism

In the first part of this thesis we explain and motivate the three main problems we want to discuss. We state two main lines on how to tackle these problems: ensemblism and individualism. Let us focus for simplicity on classical mechanics (similar arguments are made for quantum systems below). Briefly said, an ensemblist thinks of multiple copies (ensembles) of a system properly described by a probability distribution ρ on phase space Γ . While for an individualist the system is described by a single, individual phase point $X \in \Gamma$. From there on different micro states X, X' can represent the same macro state, which leads to a partition of phase space into macro regions Γ_ν . Among those is one macro region overwhelmingly large in size, associated with macroscopic thermal equilibrium Γ_{eq} . Thermalization is now understood as the evolution of a phase point through phase space according to Hamilton's equations, such that X_t spends most of its time in Γ_{eq} . Due to recurrence a statement such as $t \rightarrow \infty$ is not possible. However it is possible in the ensemblistic view, as thermalization is understood as the convergence of ρ_t to ρ_{eq} as $t \rightarrow \infty$. Although mathematically well posed, it is conceptually unclear what this means, that a phase point in thermal equilibrium is random with probability distribution ρ_{eq} . It is some-

²Most can be understood as “very probable”. We explain details below.

times claimed that this has to do with our ignorance of such a system, that its our degree of belief expressed through $\rho_{\text{eq}}(x)$ of whether $x = X$ with $X \in \Gamma_{\text{eq}}$. From an individual perspective it is much more clear what it means for a system to be in thermal equilibrium, especially since we consider a single system, say a single thermos bottle, and not a whole ensemble of it. Similar arguments can be made with respect to entropy and the second law. Further it's unclear what the very meaning of thermodynamic ensembles from an ensemblistic perspective is physically if it relies so heavily on the knowledge of an observer. It will turn out later that this is based on a wrong understanding of what probability actually means in statistical mechanics. Both views rely on statistical reasoning as its unfeasible to treat many particle systems exactly. However both views draw different consequences from that. The ensemblist by having either an “objective” frequentist view of probabilities and the “subjective” view relying on degrees of belief and knowledge. From an individualist view both are misleading, but somehow related as they can be connected through a proper typicality analysis. This means that actual distributions, that is empirical distributions are approximated in some limit (usually large particle number) with the theoretical distributions (the probabilities appearing as ensembles) by a fitting typicality measure. That is the right way to understand ensemblist. We explain details below.

As we will argue, for quantum systems, the Boltzmannian quantum framework (BQF) is the way to go. In a nutshell one could say that it's the application of the law of large numbers to systems with a large number of degrees of freedom. But still there's more. A key insight of Boltzmann was to connect the microscopic realm with the macroscopic realm. In particular by arguing that thermal equilibrium is the macro state that is realized by almost all micro states. That line of reasoning is nowadays called typicality. The typical behavior is the one that takes place in most cases. To get a first grip at the notion of typicality it is helpful to think of it in terms of probability. The typical behavior is the one that happens with very high probability, for example it is very likely that in a series of coin flips heads and tails will appear equally often. It is very likely that heat flows from a hotter to a cooler body. In the same vein: it is rather unlikely that opening the window during a cold winter night will heat up your apartment. Physics is about explaining phenomena in nature. Typicality is a way of doing that.

The classical reasoning can be applied to quantum mechanics. The aim is to understand thermal properties of a closed macroscopic quantum system with D -dimensional Hilbert space $\mathcal{H}$, in particular thermalization and the second law, from the microscopic dynamics, that is the unitary evolution of a wave function $\psi \in \mathcal{H}$, i.e.,

$$\psi_t = e^{-i\hat{H}t}\psi_0, \tag{0.1}$$

where $\hat{H}$ is the Hamiltonian and ψ_0 and initial state (we set $\hbar = 1$). By the reductionist enterprise, different micro states should represent the same macro state. Following von Neumann [297], this can be done as follows. Suppose $\hat{M}_1, \dots, \hat{M}_K$ is a family of self-adjoint operators on $\mathcal{H}$. Due to their macroscopic nature, they should be measurable simultaneously. Von Neumann claimed, that one measures operators close to $\hat{M}_1, \dots, \hat{M}_K$, that is $\hat{M}_i \approx \hat{A}_i$, such that the $\hat{A}_i$ commute pairwise. Further one argues that several microscopic eigenvalues can not be distinguished due to measurement capabilities and are collected to represent one macro value. This then leads to a decomposition of Hilbert space into orthogonal subspaces

$$\mathcal{H} = \bigoplus_{\nu} \mathcal{H}_{\nu}, \quad (0.2)$$

where each $\mathcal{H}_{\nu}$ is associated with a macro state ν . Further we write $\dim \mathcal{H}_{\nu} = d_{\nu}$ and $\hat{P}_{\nu}$ as the projector on $\mathcal{H}_{\nu}$. Among the $\mathcal{H}_{\nu}$ is a subspace that has by far the largest dimension, $d_{\text{eq}}/D \approx 1$ and is associated with thermal equilibrium $\mathcal{H}_{\text{eq}}$. A system is said to be in macroscopic thermal equilibrium (MATE) if and only if $\psi \in \mathcal{H}$ lies close to $\mathcal{H}_{\text{eq}}$, which means that

$$\langle \psi | \hat{P}_{\text{eq}} | \psi \rangle \approx 1. \quad (0.3)$$

It's a key property of thermal equilibrium, that most wave functions are in thermal equilibrium. This is a central typicality result and explains why systems are in thermal equilibrium. It's because thermal equilibrium is the macro state that is realized by most of the micro states. Here most refers to the uniform distribution on $\mathcal{H}$ (actually on the set of normalized wave functions, but due to ease of notation we simply write $\mathcal{H}$. We will be more precise below.).

Thermalization is understood as the approach to $\mathcal{H}_{\text{eq}}$. That means

$$\langle \psi_t | \hat{P}_{\text{eq}} | \psi_t \rangle \approx 1 \quad (0.4)$$

for most of the time. As mentioned due to recurrence, this can not hold for arbitrary times. Still recurrence times grow exponentially in the size of systems and are thus irrelevant. A condition ensuring that any ψ_0 approaches MATE is the eigenstate thermalization hypothesis (ETH), stating that any eigenvector of $\hat{H}$ is in MATE. For both MATE and the approach to MATE typicality statements are made, stating that most $\psi \in \mathcal{H}$ are in MATE or most $\hat{H}$ are such that the ETH is satisfied. In quantum systems, not only MATE is relevant. There are other forms of equilibrium, that can also be stated in the BQF, such as normal equilibrium, which means that most wave functions are such that for most of the time

$$\langle \psi_t | \hat{P}_{\nu} | \psi_t \rangle \approx \frac{d_{\nu}}{D}. \quad (0.5)$$

Typicality reasoning is commonly used in quantum statistical mechanics. It basically means that with very high probability certain thermal behavior appears. For this one needs probability measures. Depending on which elements of the system one is interested - among which are usually the states, Hamiltonians, Observables, times, etc. - different measures can be used. The most common and simplest one is the uniform distribution. Then a behavior is typical if it occurs with very high probability with respect to the uniform distribution. Let us however mention at this point already that although closely related, probability and typicality are of a different breed.

We now discuss more philosophical aspects. This is not surprising as fundamental aspects in physics are closely intertwined with philosophy. A fundamental question of quantum statistical mechanics is: why are systems in thermal equilibrium? The short answer is: because it's typical. That's the behaviour that most systems show. It's what thermal equilibrium means. That is, typicality allows to explain the emergent macroscopic behavior from an underlying microscopic theory. This analysis due to Boltzmann might be part of a more general framework going beyond the emergence of the second law. It does so also in Bohmian mechanics and one might be inclined to ask whether it is possible to form a more abstract framework, which could possibly yield useful insights. A key notion here is that of a primitive ontology (PO). The main idea is that it's "stuff" in three dimensional space, which makes up the macroscopic matter. Examples are for instance particle positions in Bohmian mechanics; more general one could say that a PO is what atom meant for the ancient greeks. The PO is governed by some deterministic law. Through this law the PO evolves in time. These micro-histories are epistemically accessible as they are connected to the macroscopic behavior. In particular they allow to do a statistical reasoning in form of typicality. Macroscopic behavior is explained, if typical histories of the PO account for it. Examples beneath thermalization in Boltzmannian statistical mechanics are for instance the Born rule in Bohmian mechanics. It has to be emphasized that typicality connects empirical distributions with theoretical distributions. That is, the actual distribution can be approximated with a deterministic distribution, which is then said to be the typical distribution. In this sense one can for example understand the Maxwellian velocity distribution as the typical distribution. It should be emphasized that also for quantum systems described in the orthodox setup this works. So one might think that a large number of degrees of freedom is important as well as typicality and a realist view.

Second Law in BQF

In this part we discuss the second law of thermodynamics within the BQF. There are several reasons, why this is expected to be successful. First, it works in the classical setting. Second, thermalization, i.e., the minus first law, can be well understood in

the BQF. Third, the idea of entropy increase is simple and natural in the BQF. The right notion of entropy is the quantum Boltzmann entropy

$$S_{\text{QB}}(\nu) = k_{\text{B}} \log \dim \mathcal{H}_{\nu}. \quad (0.6)$$

It is defined on the micro states $\psi \in \mathcal{H}_{\nu}$ (thus also out of equilibrium), is extensive and in thermal equilibrium given by the thermodynamic entropy. Other entropies, such as the von Neumann entropy, have flaws, as they can not account for the increase over time. Further they rely on density matrices expressing subjective ignorance. The quantum Boltzmann entropy however is defined by a pure state and therefore does not rely on any subjective knowledge.

One has to explain what it means that $S_{\text{QB}}(\nu)$ increases with time. We make two proposals, which are agnostic about the measurement problem (also known as Schrödinger's cat). We also express the second law for Bohmian mechanics.

Our first proposal looks as follows. The macroscopic history of a macro state ν is given by the superposition weights $p_{\nu}(t) = \|\hat{P}_{\nu}\psi_t\|^2$. Now for each time t these define a distribution on the set of macro states $\mathcal{N}$ and in particular a histogram with a column for each ν . We order this set along their dimension, in the sense that $\nu < \nu'$ if and only if $d_{\nu} < d_{\nu'}$. As entropy increase means that wave functions evolve from subspaces with small dimension to subspaces with larger dimension, the distribution $\|\hat{P}_{\nu}\psi_t\|^2$ has to behave such that at each later time, the columns of the histograms with larger dimension rise, while the columns of the histograms with smaller dimensions have to shrink. Thinking of histograms for several time steps, this means that the columns are moving to the right until a time T , where the system has reached MATE, i.e., $\|\hat{P}_{\text{eq}}\psi_T\|^2 \approx 1$ (see 5.1). This behavior is called right moving and allows us to state the weak second law (WSL):

WSL: For a reasonable choice of $\hat{H}$, decomposition $\mathcal{H} = \bigoplus_{\nu} \mathcal{H}_{\nu}$, initial macro state ν_0 , and initial micro state $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$, the family $(p_{\nu}(t))_{t \in [0, T]}$ is approximately right moving up to time T , where T is the time scale of reaching MATE.

A “reasonable choice” should be such that the WSL holds typically. Consider for example such a choice to be a random $\hat{H}$ with distribution $\mathbb{P}$ and arbitrary initial state ψ_0 . Then the goal is to determine the deterministic approximation $w_{\nu}(t)$ of $p_{\nu}(t)$, which are right moving. More abstractly one wants to show that

$$\mathbb{P}(|p_{\nu}(t) - w_{\nu}(t)| < \varepsilon) \approx 1, \quad (0.7)$$

for most times t and $\varepsilon > 0$.

There's another proposal for the entropy increase using a probability current. As the weights $p_{\nu}(t)$ evolve in time, probability is transported to different macro spaces.

This transport is expressed through a probability current $J_{\nu\nu'}^{\psi_0}(t)$, asserting the probability flowing from ν' to ν , depending on the initial micro state $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$. It is defined through the temporal change of the weights, i.e.,

$$\frac{d}{dt}p_\nu(t) = \sum_{\nu'} J_{\nu\nu'}^{\psi_0}(t) = \sum_{\nu'} 2\text{Im}\langle\psi_t|P_\nu H P_{\nu'}|\psi_t\rangle. \quad (0.8)$$

This allows us to formulate another version of the second law called the strong second law (SSL):

SSL: For a reasonable choice of $\hat{H}$, decomposition $\mathcal{H}_{\text{mc}} = \bigoplus_\nu \mathcal{H}_\nu$, initial macro state ν_0 , and $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$, the discrete current $J_{\nu\nu'}^{\psi_0}(t)$ points overwhelmingly from smaller $\mathcal{H}_\nu$ to larger $\mathcal{H}_{\nu'}$:

$$J_{\nu\nu'}^{\psi_0}(t) \leq 0 \quad (0.9)$$

for $t \in [0, T]$, where T is the time scale of reaching MATE.

Again a reasonable choice will be one in order to find the typical current, meaning that with very high probability

$$J_{\nu\nu'}^{\psi_0} \approx C_{\nu\nu'}(t) \quad (0.10)$$

for $t \in [0, T]$, such that $C_{\nu\nu'}(t)$ points overwhelmingly to subspaces with larger dimension.

For both, the WSL and the SSL, we will explain in detail below what the “approximate” and “overwhelmingly pointing” means. In essence one tries to quantify the degree of violation of the WSL and SSL and argue that these are negligible.

Both the WSL and SSL can be shown to hold for a Hamiltonian $\hat{H}$ given by a Wigner matrix, which is a $D \times D$ matrix $\hat{H} = (h_{ij})$ that has i.i.d. entries, with vanishing mean and variance matrix $\mathbb{E}|h_{ij}|^2 = 1/D$. In recent years these matrices have played a huge role in investigating thermal behavior of closed quantum systems with mathematical rigor (see, e.g., [63, 94, 65, 92, 61]). Let $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$ be an arbitrary initial state. We argue that for Wigner matrices the typical weights are given by

$$||\hat{P}_\nu \psi_t||^2 = \frac{d_\nu}{D} + \frac{J_1^2(2t)}{t^2} \left(\delta_{\nu\nu_0} - \frac{d_\nu}{D} \right). \quad (0.11)$$

Here $J_1(x)$ denotes the Bessel function of first kind. The precise form is not important here. At this point it is helpful that for sufficiently large times the function $(J_1(2t)/t)^2$ behaves like $1/t^3$. From there one can easily see that the weights are moving to the right and therefore fulfill the WSL. Consider for instance two macro states ν and ν' with $d_\nu < d_{\nu'}$. Further let ν_0 lie between ν and ν' . For $t = 0$, we have

$\|\hat{P}_{\nu_0}\psi_0\|^2 = 1$. Now let $t > 0$. We now compare the weights for ν with the ones for ν' . One immediately sees that

$$\|\hat{P}_\nu\psi_t\|^2 < \|\hat{P}_{\nu'}\psi_t\|^2 \quad (0.12)$$

as $d_\nu < d_{\nu'}$. That means the distribution has moved to the right.

One can also compute the current $J_{\nu\nu'}^{\psi_0}(t)$ for Wigner matrices. Let $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$ be an arbitrary initial micro state and let $\hat{H}$ be a Wigner matrix. Then the typical current is given by

$$J_{\nu\nu'}^{\psi_0}(t) = \frac{4}{D}(d_\nu\delta_{\nu_0\nu'} - d_{\nu'}\delta_{\nu\nu_0})\frac{J_1(2t)J_2(2t)}{t^2}, \quad (0.13)$$

where again $J_1(x)$ denotes Bessel function of first kind. It can be seen that probability is flowing only from ν_0 into ν or ν' . That is for entropy to increase it has to flow overwhelmingly to the larger of those two. Let $\nu_0 = \nu$ and $d_\nu < d_{\nu'}$. Then

$$J_{\nu_0\nu'}^{\psi_0}(t) = -4\frac{d_{\nu'}}{D}\frac{J_1(2t)J_2(2t)}{t^2} \leq 0, \quad (0.14)$$

which is the case for most of the times. Although violations appear quite frequently their amplitudes are small compared to the cases where it holds.

There are also other matrix models, where a WSL can be shown. These are known as Gaussian unitary ensembles. The entries of these matrices are Gaussian distributed and they are invariant under unitary transformations. They are similar to the Wigner matrices, as they give an explicit i.i.d. distribution for entries, namely the Gaussian.

We also show that for a more advanced random matrix model a WSL holds. This model has more realistic traits as the variance matrix is not constant. However it is restricted to a setting with two and three subspaces.

Further we show how a general approach using Wigner matrix models leads to expressions for the weights and the current. Key here is the use of resolvents of $\hat{H}$, expressing the unitary evolution operator $e^{-i\hat{H}t}$ using residue calculus. Finding deterministic approximations for such expressions has been key in random matrix theory in recent years for Wigner matrices (see, e.g., [63, 64]). The key difficulty is that these approximations rely on solving a non-linear equation. Solving this equation becomes more difficult, when allowing more general variance profiles $\mathbb{E}|h_{ij}|^2 = S_{ij}$ for $\hat{H} = (h_{ij})$. This however would be needed to treat more realistic systems. Possible results in the future regarding more realistic random matrix models, such as banded or sparse matrices will allow direct application for our setting.

We also propose another approximation for the weights and the current. This is related to an effective dynamics trying to derive statistical distributions for $\hat{H}$. Among those are the density of states. Among those are also distributions, which capture

the statistics of the overlaps among different macro states with energy eigenvectors as these appear naturally in the weights and the current. Ultimately smoothed out versions of these empirical distributions allow to replace sums with integrals and get an effective dynamics.

Finally, we discuss how the second law can be stated in Bohmian mechanics. Orthodox quantum mechanics has a severe issue: the measurement problem. It is solved by appealing to a collapse of the wave function, whenever some measurement is made. However it's not clear what exactly this means and what role an observer plays. In so called quantum theories without observers the measurement problem is solved. We particularly focus on Bohmian mechanics. It's a non-relativistic quantum theory, which is about point like particles having positions Q in three dimensional space, and their evolution in time is governed by a guiding equation that contains the wave function ψ , which itself follows the Schrödinger equation. We think of a macro state ν_t as given by the pair $\nu_t = (Q(t), \psi_t)$. Since $Q(t)$ is random with probability density $|\psi_t|^2$, the evolution of ν_t will be a stochastic process on the set of macro states. The Markovization of that process is a Bell process. A Bell process is a jump process with certain jump rates. In our case this means that $(\nu_t)_{t \in \mathbb{R}}$ defines a jump process on $\mathcal{N}$, which means that transitions from ν' to ν are given by

$$\sigma_t(\nu' \rightarrow \nu) = \frac{[J_{\nu\nu'}(t)^{\psi_0}]^+}{\|\hat{P}_{\nu'}(t)\|^2}, \quad (0.15)$$

where $x^+ = \max(0, x)$ denotes the positive part. That means for a reasonable choice (as above for the WSL and SSL) one can formulate a Bell second law, which states there are overwhelmingly more transitions from smaller ν to larger ν' , i.e., $\sigma_t(\nu \rightarrow \nu') \gg \sigma_t(\nu' \rightarrow \nu)$. We show that this is the case for Wigner matrices. Similar considerations are expected to hold for Wigner-type matrices, which have a more general (non-constant) variance profile.

Thermal Equilibrium of Subsystems

In the third part, we explain how wave functions properly describe thermal equilibrium of subsystems and thus support the individualistic view. This is based on the work [148] (see Appendix 11.2). We will discuss certain aspects in more detail.

First, we discuss the relevant notions to describe thermal equilibrium for systems composed of a subsystem S and a heat bath B . Let $\mathcal{H}^S$ and $\mathcal{H}^B$ denote the respective Hilbert spaces of S and B , such that the total Hilbert space of $S \cup B$ is given by $\mathcal{H} = \mathcal{H}^S \otimes \mathcal{H}^B$. There are two ways to assign a state to S : one through density matrices and one through wave functions. We start with the former.

A density matrix $\hat{\rho}$ arises either as a statistical operator, that is for $\Psi \sim \mu$, with a

probability measure μ , and are given by a “mixture” $\hat{\rho}_\mu = \mathbb{E}|\Psi\rangle\langle\Psi|$ (where $\mathbb{E}$ denotes the expectation value with respect to μ and which should be clear from the context) or as a reduced density matrix $\hat{\rho}^S = \text{tr}^B \hat{\rho}$, where the degrees of freedom of B have been traced out. We are especially interested in the reduced density matrices for pure states $\Psi \in \mathbb{S}(\mathcal{H})$ of the total system

$$\hat{\rho}_\Psi^S := \text{tr}^B |\Psi\rangle\langle\Psi|. \quad (0.16)$$

A wave function is assigned to a subsystem S as follows. Let $\Psi \in \mathcal{H}$ be a wave function of $S \cup B$. Let $b = \{|b_1\rangle, |b_2\rangle, \dots\}$ be an orthonormal basis (ONB) of $\mathcal{H}^B$, then the conditional wave function

$$\psi^S = \mathcal{N} \langle b_J | \Psi \rangle_B \quad (0.17)$$

is a random element of $\mathcal{H}^S$ with normalization constant $\mathcal{N}$, the partial inner product $\langle \cdot | \cdot \rangle$ and the basis element b_J chosen with quantum probability $\mathbb{P}(J = j) = \|\langle b_J | \Psi \rangle_B\|_S^2$. One can think of ψ^S as the collapsed wave function after an ideal quantum measurement of b on the heat bath B .

We now discuss how both state assignments describe thermal properties of S . Thermodynamic ensembles, such as the canonical or grand-canonical ensemble appear by tracing out the micro-canonical density matrix $\hat{\rho}_{\text{mc}}$ of the total system $S \cup B$. That means if the total system $S \cup B$ is in thermal equilibrium (at temperature T), then for B large enough (such that T does not change significantly), the state of S is given by the well known canonical density matrix $\hat{\rho}_{\text{can}}$.

Another - conceptually stronger - way to obtain this result has been proposed by several groups [108, 214, 133] and is nowadays known as “canonical typicality”. Briefly, it states that for most wave functions $\Psi \in \mathcal{H}_{\text{mc}}$ (where most is referred to the uniform distribution over the sphere $\mathbb{S}(\mathcal{H}_{\text{mc}})$), where $\mathcal{H}_{\text{mc}} \subset \mathcal{H}$, the reduced density matrix in the thermodynamic limit is canonical, i.e.,

$$\text{tr}^B |\Psi\rangle\langle\Psi| \approx \hat{\rho}_{\text{can}}. \quad (0.18)$$

The statement just mentioned for the canonical ensemble is again a typicality statement.

Canonical typicality is a purely quantum phenomena, having its roots in entanglement: Ψ is a pure state, but $\hat{\rho}_{\text{can}}$ is not, it is mixed (in general it has many different non-zero eigenvalues, i.e., $\hat{\rho}_{\text{can}}^2 \neq \hat{\rho}_{\text{can}}$). Classically this is not the case as tracing out degrees of freedom of a phase point $X = (X_S, X_B)$ simply yields another phase point X_S (and not a probability density).

A central aspect is that canonical typicality shows that pure states can mimic thermal behavior. What canonical typicality actually shows (as $\text{tr}^B \hat{\rho}_{\text{mc}} \approx \hat{\rho}_{\text{can}}$ by

standard conceptually harmless arguments) is that for most $\Psi \in \mathcal{H}_{\text{mc}}$ one finds

$$\text{tr}^B |\Psi\rangle\langle\Psi| \approx \text{tr}^B \hat{\rho}_{\text{mc}} \quad (0.19)$$

That means for a suitable self-adjoint operator $\hat{A}$ most pure states yield exactly the same statistics as the micro-canonical density matrix, that is

$$\mathbb{E}\langle\Psi|\hat{A}|\Psi\rangle \approx \text{tr}(\hat{A}\hat{\rho}_{\text{mc}}). \quad (0.20)$$

One can show that this is the case not only for most wave functions on the energy shell, but also on more general subspaces which arise under some given constraint. It is this fact, and this fact alone, that justifies the micro-canonical distribution: thermodynamic ensembles appear typically.

In the literature there are roughly two common views justifying the thermodynamic ensembles. That is by appealing to the principle of equal a priori probabilities or to the maximum entropy principle. We argue that both views are misleading, because they rely on a wrong understanding of probabilities involving the role of an observer and his knowledge. We believe that it is a fact of nature how systems behave in thermal equilibrium and that this is explained by the notion of typicality. It's simply typical that they behave as described by the thermodynamic ensembles. Once a behavior is coined as typical there is nothing left to explain. It's exactly the behavior that happens *in nature*.

In the same vein (and somehow connected) to canonical typicality is the question whether the random wave function ψ^S has a particular thermal equilibrium distribution. This has been motivated in [134, 132] as a quantum analogy to classical thermodynamic ensembles. In the latter thermal equilibrium means that a phase point X of a subsystem S has probability density $\rho_{\text{can}}(x)$ or more general a probability measure μ_{can} , i.e., $X \sim \mu_{\text{can}}$. For quantum mechanics this means whether there are thermal equilibrium measures μ_{eq} , such that in thermal equilibrium $\psi^S \sim \mu_{\text{eq}}$. Note however, that in classical mechanics thermal equilibrium just described is understood ensemblistically, while here for wave functions we have a more individualistic view.

A problem arising is this: wave functions are normalized that is they are elements of the unit sphere $\mathbb{S}(\mathcal{H})$, which we denote as

$$\mathbb{S}(\mathcal{H}) := \{\psi \in \mathcal{H} : \|\psi\| = 1\}. \quad (0.21)$$

The wave function of an open quantum system has the GAP measure as its universal distribution in thermal equilibrium. More precisely, if the heat bath B is large, then for most ONBs b of $\mathcal{H}^B$ and most $\Psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$, the subsystem wave function ψ^S is approximately $\text{GAP}_{\hat{\rho}_{\text{can}}}$ -distributed for suitable inverse temperature $\beta = \beta(E)$. Note

that $\text{GAP}_{\hat{\rho}_{\text{can}}}$ should be seen as the distribution of wave functions in the canonical ensemble. A better example is the micro-canonical density matrix as it is associated with $\text{GAP}_{\hat{\rho}_{\text{mc}}}$, which is the uniform measure $u_{\mathbb{S}(\mathcal{H}_{\text{mc}})}$ over $\mathbb{S}(\mathcal{H}_{\text{mc}})$. That is there is a particular universal distribution *in nature* for a wave function ψ^S of S in thermal equilibrium. It has nothing to do with our ignorance.

Let us discuss the GAP measure more closely. GAP measures are a family of probability measures on the unit sphere $\mathbb{S}(\mathcal{H})$. The acronym GAP stands for Gaussian, Adjusted and Projected measure. As wave functions lie on the unit sphere one has to properly adjust and project the measure such that its defined on $\mathbb{S}(\mathcal{H})$. More generally, any density matrix $\hat{\rho}$ on $\mathcal{H}$ has $\text{GAP}_{\hat{\rho}}$ as its associated probability measure on the unit sphere $\mathbb{S}(\mathcal{H})$. It has universal status among all μ on $\mathbb{S}(\mathcal{H})$ with density matrix (covariance) $\hat{\rho}$. Therefore $\text{GAP}_{\hat{\rho}}$ can be seen as the most spread out distribution over the unit sphere $\mathbb{S}(\mathcal{H})$ with density matrix $\hat{\rho}$.

We extend the above results to the grand-canonical setup. That is not only an extension of canonical typicality and the GAP measure to the grand-canonical case. To this end we make use of the generalized Gibbs ensemble

$$\hat{\rho}_{\text{gG}} = Z_{\text{gG}}^{-1} \exp \left(\sum_{k=1}^K \lambda_k \hat{Q}_k \right), \quad (0.22)$$

which arises for a system that involves multiple conserved quantities $\hat{Q}_1, \dots, \hat{Q}_K$ (besides energy and total particle number); here $\lambda_1, \dots, \lambda_K$ is a family of parameters. To this end one has to consider a subspace $\mathcal{H}_{\text{gmc}}$ called “generalized micro-canonical subspace” of the total Hilbert space $\mathcal{H}$ to which the system is confined due to the conserved observables:

$$\mathcal{H}_{\text{gmc}} := \text{span} \left\{ \phi \in \mathcal{H} : \forall k : \hat{Q}_k \phi = q_k \phi, q_k \in [Q_k - \Delta Q_k, Q_k] \right\}. \quad (0.23)$$

For $\mathcal{H}_{\text{gmc}}$ one can assign the normalized projection $\hat{\rho}_{\text{gmc}} = \hat{P}_{\text{gmc}}/d_{\text{gmc}}$ with projector $\hat{P}_{\text{gmc}}$ onto $\mathcal{H}_{\text{gmc}}$ and $d_{\text{gmc}} = \dim \mathcal{H}_{\text{gmc}}$.

Further let $\Lambda \subset \mathbb{R}^3$ and S be a spatial region in Λ with $\bar{S} = \Lambda \setminus S$. Let $\mathcal{H}^\Lambda$ be a Hilbert space for each $S \subseteq \Lambda$ and let $\mathcal{H}^S$ be such that for $S_1 \subseteq S_2 \subseteq \Lambda$ we have $\mathcal{H}^{S_2} = \mathcal{H}^{S_1} \otimes \mathcal{H}^{S_1 \setminus S_2}$. Further let $\hat{Q}_1, \dots, \hat{Q}_K$ be a set of lower bounded self-adjoint operators, which commute pairwise and are approximately extensive, that is $\hat{Q}_k \approx \hat{Q}_k^S \otimes \hat{I}^{\bar{S}} + \hat{I}^S \otimes \hat{Q}_k^{\bar{S}}$. As a consequence $\hat{\rho}_{\text{gG}} \approx \hat{\rho}_{\text{gG}}^S \otimes \hat{\rho}_{\text{gG}}^{\bar{S}}$. We denote the eigenvalues of $\hat{Q}_k$ as Q_k .

We first show that for $\lambda_1, \dots, \lambda_K$ satisfying $\text{tr}(\hat{\rho}_{\text{gG}} \hat{Q}_k) = Q_k$, large enough $\mathcal{H}_{\text{gmc}}$ and small $S \subset \Lambda$, that

$$\text{tr}^{\bar{S}} \hat{\rho}_{\text{gmc}} \approx \hat{\rho}_{\text{gG}}^S. \quad (0.24)$$

This can be seen as a generalization of the standard textbook derivation for the canonical or the grand-canonical ensemble (think of the $\hat{Q}_k$ as the Hamiltonian or the particle number operator).

Considering $\mathcal{H}_{\text{gmc}}$ allows us to go beyond the textbook derivation of the grand-canonical ensemble as it also takes chemical reactions into account and not only the scenario where particles enter or leave a spatial region S . One really has to emphasize the role of the conserved observables $\hat{Q}$ here as for a chemical reaction, say $A + B \rightleftharpoons C + \delta E$ (here δE is the energy released or consumed during the reaction) the total particle number of each species is not conserved, but certain linear combinations of them are; in the example $\hat{Q}_1 = \hat{N}_A - \hat{N}_B$ and $\hat{Q}_2 = \hat{N}_A + \hat{N}_C$ are conserved. Doing so, we justify what the average number of each particle species in thermal equilibrium is and compute the chemical potential arriving at what one would expect from a standard textbook treatment.

We also show that $\hat{\rho}_{\text{gG}}$ is universal. In similar spirit, but a different setup we also show that the grand-canonical ensemble is universal; see Appendix 11.2. Extending canonical typicality, we use results from [214] to derive ensemble typicality: most pure states $\Psi \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$ are such that the reduced density matrix of a small region $S \subset \Lambda$ is approximately a generalized Gibbs density matrix: $\hat{\rho}_{\Psi}^S := \text{tr}^{\bar{S}} |\Psi\rangle\langle\Psi| \approx \hat{\rho}_{\text{gG}}^S$. In particular we show that $\hat{\rho}_{\text{gG}}^S$ does not rely on the maximum entropy principle.

We further argue that for a small region $S \subset \Lambda$ most $\Psi \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$ and most ONBs b of $\mathcal{H}^B$ are such that the conditional wave function ψ^S has as $\text{GAP}_{\hat{\rho}_{\text{gG}}^S}$ as its thermal equilibrium distribution for large enough B .

A novelty about GAP measures is this: for a basis b , which is typical among those ONBS, which diagonalize $\hat{Q}_1^{\bar{S}}, \dots, \hat{Q}_{K-1}^{\bar{S}}$ (excluding $\hat{H}^{\bar{S}}$) and $\hat{N}_i^{\bar{S}}$ leads to mixtures of GAP measures with certain coefficients given by the Born distributions. Then for $S \subset \Lambda$ small, most $\Psi \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$ and most ONBs b of $\mathcal{H}^{\bar{S}}$ diagonalizing $\hat{Q}_1^{\bar{S}}, \dots, \hat{Q}_{K-1}^{\bar{S}}$ are such that

$$\psi^S \sim \mathbb{P}_{\text{gG}} \bigoplus_{q_1^S, \dots, q_{K-1}^S} p(q_1^S, \dots, q_{K-1}^S) \text{GAP}_{\hat{\rho}^S(q_1^S, \dots, q_{K-1}^S)} \quad (0.25)$$

for large enough $\bar{S}$ where

$$p(q_1^S, \dots, q_{K-1}^S) = \text{tr}(\hat{\rho}_{\text{gG}}^S \hat{P}) \quad \text{and} \quad \hat{P} = \hat{P} \left(\hat{Q}_1^S = q_1^S, \dots, \hat{Q}_{K-1}^S = q_{K-1}^S \right) \quad (0.26)$$

and

$$\hat{\rho}^S(q_1^S, \dots, q_{K-1}^S) = \frac{1}{p(q_1^S, \dots, q_{K-1}^S)} \hat{P} \hat{\rho}_{\text{gG}}^S \hat{P}. \quad (0.27)$$

Here we denote

$$\hat{P}(\hat{A}_1 = a_1, \dots, \hat{A}_r = a_r) \quad (0.28)$$

for the projection to the joint eigenspace of commuting $\hat{A}_1, \dots, \hat{A}_r$ with eigenvalues $a_1, \dots, a_r$. By the Born rule, the joint probability distribution of the outcomes in a simultaneous quantum measurement of the observables $\hat{A}_1, \dots, \hat{A}_r$ on a system with density matrix $\hat{\rho}$ is given by

$$\mathbb{P}(\hat{A}_1 = a_1, \dots, \hat{A}_r = a_r) = \text{tr} \left[\hat{\rho} \hat{P}(\hat{A}_1 = a_1, \dots, \hat{A}_r = a_r) \right]. \quad (0.29)$$

We also explain the approach to thermal equilibrium of S . Assume that $\hat{H}$ satisfies the eigenstate thermalization hypothesis (ETH), which means that for two distinct energy eigenstates $\phi_n, \phi_m \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$

$$\text{tr}^{\bar{S}} |\phi_n\rangle\langle\phi_m| \approx \delta_{nm} \text{tr}^{\bar{S}} \hat{\rho}_{\text{gmc}}. \quad (0.30)$$

Then every initial state $\Psi_0 \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$ will for most $t \geq 0$ be such that

$$\hat{\rho}_{\Psi_t}^S \approx \text{tr}^{\bar{S}} |\Psi_t\rangle\langle\Psi_t| \approx \hat{\rho}_{\text{gG}}^S \quad (0.31)$$

and also for $\hat{\rho}_{\text{gc}}^S$.

Further every initial state $\Psi_0 \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$, for most ONBs b , for most times $t \geq 0$, the conditional wave function $\psi^S(t)$, which arises from the time dependence of Ψ_t is roughly distributed by its thermal equilibrium measure, that is by GAP $\hat{\rho}_{\text{gG}}^S$.

The upshot is that results on ensemble typicality and GAP measures, particularly in the case of generalized Gibbs ensembles, support the individualistic picture in which pure states themselves display the relevant thermal behavior in nature.

Part I.

**Foundations of Statistical
Mechanics**

1. Three Fundamental Problems of Quantum Statistical Mechanics

The corner stones of modern physics, developed in the last 150 years are statistical mechanics, general relativity and quantum mechanics. Statistical physics deals with systems that have a large number of degrees of freedom trying to derive essential macroscopic features of such systems without taking all microscopic details into account. By doing that it has been extremely successful from the smallest to the largest scales in the universe (see, e.g., [176, 44, 56, 9, 116]).

Still not everything is settled as fundamental questions remain, in particular regarding the derivation of the laws of thermodynamics from quantum mechanics as well as the justification of thermodynamic ensembles for closed macroscopic quantum systems. The main aim of this thesis is to propose answers to these questions.

We consider a closed macroscopic quantum system $\mathcal{S}$ in some finite volume $\Lambda \subset \mathbb{R}^3$, with Hilbert space $\mathcal{H}$ and discuss how thermal equilibrium, thermalization and the increase of entropy can properly be described by a wave function $\psi \in \mathbb{S}(\mathcal{H})$ lying in the unit sphere $\mathbb{S}(\mathcal{H}) := \{\psi \in \mathcal{H} : \|\psi\| = 1\}$ evolving unitarily

$$\psi_t = e^{-i\hat{H}t}\psi_0 \quad (1.1)$$

with initial wave function $\psi_0 \in \mathbb{S}(\mathcal{H})$, according to the Schrödinger equation

$$i\frac{\partial\psi_t}{\partial t} = \hat{H}\psi_t, \quad (1.2)$$

where $\hat{H}$ is the Hamiltonian (we set $\hbar = 1$, if not stated otherwise). Here we focus on “abstract” systems, which means that instead of considering Hamiltonians of the form

$$\hat{H} = -\frac{1}{2m} \sum_{i=1}^N \Delta_i + \sum_{i<j} \hat{V}(|\mathbf{q}_i - \mathbf{q}_j|), \quad (1.3)$$

with Laplace operator Δ_i acting on the i -th coordinate and suitable pair potential $\hat{V}$ (e.g., Coulomb interaction), we look at generic Hamiltonians and wave functions that lie in the unit sphere $\mathbb{S}(\mathcal{H})$ (instead of a particular L^2 -space); further we consider

non-relativistic systems³.

We elaborate the role of wave functions regarding thermal equilibrium of subsystems and also the approach towards it. Consider a macroscopic quantum system $\mathcal{S}$ with a subsystem S and a heat bath B . Now the state of S is commonly described by a reduced density matrix. We will see that thermal equilibrium is well defined for pure states ψ of the total system $S \cup B$ and that “most” of these states yield the same statistics of measurement outcomes as the thermodynamic ensembles. One can also assign a wave function to S and show that such wave functions have proper universal distributions in thermal equilibrium.

Such considerations date back to the early days of quantum mechanics, in particular to the works of von Neumann [297] and Schrödinger [239, 241] highlighting the role wave functions play in describing thermal behavior. These ideas have attracted interest in the last 20 to 30 years due to key theoretical insights, such as the eigenstate thermalization hypothesis (ETH) [77, 258] and canonical typicality [133, 214, 108, 269]. It is a key insight of these works that a pure state describes the thermal behavior of systems and has lead to a large body of subsequent research on quite generic systems [272, 109, 110, 217, 266, 218, 228, 180, 219, 131, 230, 221, 127, 128, 73, 72, 224, 277, 278, 279] and also recently on a concrete model of free fermions [249, 273, 275, 232, 274, 144]. Concerning thermal properties of subsystems S embedded into a larger heat bath substantial results have been obtained by assigning thermal distributions to wave functions of a subsystem S via so called $\text{GAP}_{\hat{\rho}}$ measures [156, 134, 132, 279, 192, 296, 196, 218, 290, 291]. These $\text{GAP}_{\hat{\rho}}$ measures serve as quantum analogs of the thermodynamic ensembles in classical statistical mechanics. Further they are the most spread out measure on $\mathbb{S}(\mathcal{H})$ with density matrix $\hat{\rho}$.

Also experimental results on closed quantum systems and related topics have gained increasing interest in recent years (see, e.g., [202, 116, 45] and the cited references therein). Prominent examples include experiments with ultracold atoms [140, 283, 158, 137, 190, 23, 168] as well as studies related to the generalized Gibbs ensemble [167](see Appendix 11.2 and Part III). Numerical investigations have also been carried out (see, e.g., [202, 116] and the cited references therein). In this work, we are primarily interested in the theoretical and conceptual aspects of the above-mentioned questions; for general overviews see [202, 116, 90, 9].

In order to derive macroscopic properties one might be inclined to simply solve Schrödinger’s equation. As it turns out this problem becomes incredibly hard with an increasing number of particles; let alone for realistic systems with 10^{23} particles. Thus such an approach is neither possible nor is it needed as it might not even be relevant for understanding such systems to solve the equations of motion. It turns out that macroscopically these systems evolve according to some simple laws and that few

³One could also consider relativistic systems, see [9, p.62].

variables are enough to characterize a system and understand it reasonably well for everyday practice; these are for instance temperature, pressure, magnetization and so on [58]. A promising analysis turned out to be a *statistical analysis* of the microscopic dynamics (given initial constraints), roughly speaking by appealing to probabilistic reasoning.

Understanding macroscopic behavior from an underlying microscopic theory is a quite old endeavour dating back to the work of Daniel Bernoulli in 1731 trying to explain pressure based on the dynamics of particles. This result can be seen as a starting point of kinetic theory of gases [292, p.8]. Afterwards Boltzmann developed his famous equation [27], showing that entropy in a dilute gas never decreases and approaches the Maxwellian distribution in equilibrium [28]. The validity of this approach has mathematically been established by Lanford [166] and has been further worked out quite recently [76]. Above all that is the goal to understand the emergence of the second law of thermodynamics as formulated by Clausius [68, 69]. While Maxwell [195] realized the relevance of probabilistic reasoning for the second law, he also introduced in 1878 what later became known as ensembles [181, p.196] and worked out in more detail by Gibbs [115]. It was ultimately Boltzmann who resolved the problem of irreversibility in classical mechanics by appealing to typicality reasoning, saying that “most” initial states evolve such that entropy increases. Boltzmann’s reasoning has prevailed and we will follow it. For more on the very interesting historical development see [46, 181, 292].

There is a whole plethora of proposals on how to tackle the approach to thermal equilibrium, the definition of thermal equilibrium or the definition of entropy and its increase (see, e.g., [121, 136, 32]). Still a rough line can be drawn between approaches towards statistical mechanics.

The divide lies between ensemblists and individualists or in other words between the Gibbsian view (see, e.g., [281, 151, 163, 299, 300, 212, 142, 105, 301]), a view taken in most textbooks (see, e.g., [146, 244, 11, 10]) and those that follow the individualistic or Boltzmannian account (see, e.g., [9, 58, 177, 175, 121, 272, 128, 136, 188])⁴. It is agreed upon, both by the ensemblist and the individualist, that the derivation of macroscopic properties from an exact solution of the underlying microscopic evolution equations is impossible. Both views draw the conclusion to appeal to probabilistic reasoning. However, although using the standard formalism of probability theory, they differ in their understanding of probability (we will explain this below). The ensemblist understands it in terms of either “objective” or “subjective” probability (see, e.g., [105, 34, 9]), while the individualist understands it in terms of typicality. That has another aspect as both frameworks relate to severely different scientific frameworks. Stated differently, those that rely on a “subjective” view and those that

⁴As is often the case with the suffix “-ism,” one must ask whether the person from whom the label is derived would have described themselves in these terms.

rely on an “objective” view. One could also say positivistic attitudes against realistic attitudes.

For the Gibbsian thermal properties of a system are properly described by a suitable statistical state, a probability distribution over phase space or a density matrix in Hilbert space, while the Boltzmannian means that thermal properties of a system are properly described by a suitable pure state, a point in phase space or a wave function in Hilbert space.

We are in favor of Boltzmann’s framework and argue that relevant questions about the thermal properties of closed quantum systems find reasonable answers there. This will run through the entire thesis.

There is however no consent about what probability actually means. Does it mean chance or likelihood? Is it subjective or objective? Is it related to frequencies or is about degrees of belief? Here’s a possible answer

“A variety of notions of probability, playing different roles, are relevant in physics. One crucial notion, typicality, while not genuinely probabilistic at all, is arguably the mother of them all.”([120], p.1)

Following Goldstein, we will see that typicality is the way to go [306, 169]. It connects empirical means with theoretical means via a typicality measure. A simple example is the law of large numbers, while a more physical related example is the Maxwellian distribution of velocities, which we both explain below.

It is also important to note that this shows that there is no intrinsic randomness:

“The relevant typicality results express objective facts about the modal structure of the laws. These modal facts come with certain normative implications for what we should expect or consider to be explained, but they are not themselves of an epistemic nature.”[169, p.10]

The questions above are very conceptual and have stipulated a lot of investigations in philosophy of physics (see, e.g., [86, 4, 55, 54, 52]). First and foremost about the very meaning of probability in statistical mechanics, which we also discuss throughout this thesis and whether probability is understood as “subjective”, i.e., entropy understood as a measure of ignorance, or “objective” in the sense of frequentism (see, e.g., [9, 34, 255, 169, 105, 301]). Time reversibility or the arrow of time are in itself interesting topics for philosophical research [4]. With respect to the second law of thermodynamics the essence of thermal equilibrium has been explained by Boltzmann appealing to typicality. We usually consider boxes that are prepared in a low entropy state (well isolated) and then left to evolve. If we move that further we do not only care about boxes, but about the universe as whole and get to the “hard part” [119] of the problem of irreversibility, that is to explain the origin of the low entropy initial state. Boltzmann himself [30] made the so called “fluctuation hypothesis” (see, e.g., [284, Sec.9.2]), while it was Feynman [102, p.116] who considered the low entropy initial state as a law of nature:

“Therefore I think it is necessary to add to the physical laws the hypothesis that in the past the universe was more ordered, in the technical sense, than it is today — I think this is the additional statement that is needed to make sense, and to make an understanding of the irreversibility. ”

This lead Albert [4] to his proposal for the past hypothesis (PH); for a discussion of the PH see [49, 50, 51]. Further as the PH is posited as a law of nature, which is not of dynamical character has lead to research on the status of laws of nature [53, 54]. Note that there are also proposals without positing a PH [171].

There are also more general questions: what is the status of a macroscopic law if it only holds for most initial conditions? (see [169, 170] for a discussion). Further as typicality serves as an explanatory scheme the relation to the debate on what explanations count as scientific is also entailed [305].

As knowledge plays such a huge role in the ensemblistic view one might ask what the role of knowledge is in a physical theory. Should it play a role? Or stated differently: in what sense should it play a role? We certainly use it as we observe regularities which we remember and therefore know about. But our knowledge is not essential for phenomena to happen in nature, which we then can observe. One might also consider to discuss realistic and positivistic attitudes in foundational aspects of statistical mechanics. In particular for quantum systems, and the appearance of macroscopic superpositions, famously known as Schrödinger’s cat [9, 136]. Another aspect to mention is that micro on macro supervenience leads to interesting questions about emergent behavior and the role typicality plays there [58, 57, 56].

We now state three fundamental problems, which we discuss in this thesis. Note that in this Chapter we illustrate some of the views with quite lengthy quotes. However, this gives a solid view on how people think about these issues.

1.1. Conceptual Framework

In a very recent book on foundations of statistical mechanics Frigg and Werndl say that statistical mechanics

“has not yet found a generally accepted theoretical framework, let alone a canonical formulation.”[105, p.3]

and similar statements have been made earlier by Sklar

“[N]o single, coherent, and clear understanding as to just what the theory of statistical mechanics *is* or ought to be.”[255, p.5]

and also Jaynes

“there is no line of argument proceeding from the laws of microscopic mechanics to macroscopic phenomena that is generally regarded by physicists as convincing in all respects”[152]

1. Three Fundamental Problems of Quantum Statistical Mechanics

Similar statements can be found in [292], [116, p.44].

What might seem as something not expected among physicists from the outside is actually not surprising for the working physicist from the inside, especially regarding foundational issues: an ongoing debate and divide about how to approach a problem in the right way, here statistical mechanics.

If there is no consensus does that mean that statistical physics is just some amalgamation of several proposals all being “right” to some degree. Certainly not. Let us quote an authority from outside of physics, former Pope Benedikt, who said⁵

“Truth is not determined by a majority vote.”

We argue that the Boltzmannian framework is the way to go and that Boltzmann’s reasoning provides explanations such that a theory can be considered to be true (we will discuss this below). It turns out that asking the right question is even as good as giving a good answer, and maybe even yields the true answer. What we mean by this is that questions should be stated such that they rely on an realistic view, instead of a subjective view.

Now, as we already mentioned, there is one main divide in statistical mechanics, which lies between ensemblists and individualists. We will discuss this more in a minute. As we briefly stated above they have different views on how to understand the role of probabilistic reasoning in statistical physics. Therefore they also ask different questions about thermal equilibrium, thermalization, the second law and so on. The ensemblist thinks of systems being represented by probability distributions or more general a statistical state and therefore asks questions of the form

What is the probability distribution on the set of micro states for a system in thermal equilibrium?

The individualist does not think in terms of distributions, but of *actual* states that a system has and thus asks the relevant question:

What is the essence of a system being in thermal equilibrium?

We will see that along the tradition of Boltzmann such questions can be asked referring to typicality. It’s simply typical that systems are in thermal equilibrium (in the same way that heads and tails appear equally often in a series of coin tosses). It’s how most of the systems behave (of course our world is not in thermal equilibrium and thus not typical, but that is a different story (see, e.g., [119, 169, 4])).

⁵This is not exactly what he said, but it’s more on point. Here’s the original quote: “truth draws strength from itself and not from the number of votes in its favour.” Also what the Pope had in mind is not what we have in mind here, as physics is still a different breed than politics. See https://www.vatican.va/content/benedict-xvi/en/speeches/2006/march/documents/hf_ben-xvi_spe_20060318_intern-organizations.html, last accessed on december 14, 2025.

Although it has been confessed in the same book by Frigg and Werndl from above that the Boltzmannian approach for classical statistical mechanics is conceptually very promising, they still feel that something more important has to be said, namely this

“But the crucial question is whether, and if so how, a quantum version of BSM [Boltzmannian Statistical Mechanics, C.I.] can be formulated.” [105, p.46]

We will argue that this is the case. There exists already a well posed formalism for non-relativistic quantum mechanics in the Boltzmannian sense (see, e.g., [128, 136]). Its conceptually clear and in particular able to derive the minus first law of thermodynamics from the underlying microscopic unitary evolution [131, 232]. What has not been formulated so far is a derivation of the second law of thermodynamics; and that is maybe what Frigg and Werndl have in mind above. A conjecture has been made by Goldstein et al. [136], but not developed further. We will introduce novel proposals for the second law in Part II.

But first we describe the two main lines of thought on how to approach the conceptual problems of statistical mechanics mentioned above. Let us start with the common view: ensemblism.

In the ensemblistic view the state of a system with a large number of degrees of freedom⁶ is given by a statistical state, since

“[v]ery often, and this is the case in statistical mechanics, we only know the probabilities of finding the system in a given state.”[173, p.49]

That leads to a whole collection of identical copies of a system, therefore this approach is called **ensemblism** (see, e.g., [105, 11, 121]). Here’s Gibbs:

“We may imagine a great number of systems of the same nature, but differing in the configurations and velocities which they have at a given instant [...] we may set the problem, not to follow a particular system through its succession of configurations, but to determine how the whole number of systems will be distributed among the various conceivable configurations and velocities at any required time [...]”[115, p.vii]

Such an ensemble leads to the notion of a probability density $\rho(x)$ on phase space Γ or to a density matrix $\hat{\rho}$ (a “statistical mixture”) on Hilbert space $\mathcal{H}$ as the fundamental description of a many particle system. It is common to understand the statistical state as representing the knowledge of an observer about a system:

⁶Sometimes we loosely say “many particle system”, but that is only well defined in Boltzmann’s classical setting and Bohmian mechanics. Otherwise, for example in orthodox quantum mechanics its just loose talk as there are no particles.

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“that a whole ensemble of possible dynamic states corresponds to the same macroscopic state, compatible with our knowledge. Thus the fundamental concept of statistical ensembles of systems, is introduced quite naturally and, with it, that of a probability density defining a statistical weight for the various systems in the ensemble. The method of statistical mechanics will thus consist in associating with each macroscopic observation a certain representative ensemble of virtual systems, which are independent of one another, and in adding to these ensembles a probability density in phase in the classical theory, or a statistical operator or density matrix in the quantum theory.” [151, p.xvii]

From the ensemblist view a system is in thermal equilibrium if the density matrix is “close” to one of the thermodynamic ensembles [159, 163, 164, 189, 233, 281, 151], for example:

$$\hat{\rho} \approx \hat{\rho}_{\text{mc}} \quad \text{or} \quad \hat{\rho} \approx \hat{\rho}_{\text{can}}. \quad (1.4)$$

The Gibbsian tries to argue that the so called ensemble average (an average over all copies of the same single system)

$$\text{tr}(\hat{\rho}\hat{A}) = A_{\text{eq}} \quad (1.5)$$

yields correct thermodynamics values, say A_{eq} for an observable $\hat{A}$ of a single system, where $\hat{\rho}$ is either $\hat{\rho}_{\text{can}}$ or $\hat{\rho}_{\text{mc}}$. These averages are “the only quantities which, from the point of view of statistical mechanics, are accessible to macroscopic observations”[151, p.11].

Here density matrices are understood as “statistical mixtures”. For a wave function $\psi \in \mathbb{S}(\mathcal{H})$ distributed according to some probability measure μ on $\mathbb{S}(\mathcal{H})$, the density matrix reads

$$\hat{\rho}_{\mu} = \mathbb{E}|\psi\rangle\langle\psi|, \quad (1.6)$$

where the expectation value $\mathbb{E}$ is taken with respect to μ . In the ensemblist view the measure μ is the “subjective” probability, i.e., $\hat{\rho}_{\mu}$ expresses the degree of belief that the system has wave function ψ .

Remark 1.1.1 (Classical Ensembles). Classically a system is in thermal equilibrium if its microstate X is random (in whatever sense), with probability density (and respective probability distribution) given by one of the thermodynamic ensembles [121]. Following that view it means that the exact microstate X is not known and can not be known exactly due its randomness. A fact hard to believe as it seems hard to doubt that there is a particular state in nature corresponding to a point in phase space, which describes the system properly and not a probability distribution doing that. $\diamond$

But why should our knowledge be relevant? Does it mean that we measured the temperature of the system and realized that its roughly equal across the system. Or

does it mean that we have no epistemic access to the system (say there's a barrier and we can not "look"). Assume for a moment⁷ that our knowledge is represented by a probability density ρ_{know} . Then one is not asking if ρ_{know} is close to, say the canonical distribution [128]. Further ρ_{know} is usually widely spread, as anything could be the case or we simply don't know. Further it is not obvious what different observers conclude, since they clearly have different knowledge and thoughts (see, e.g., [34, 188]). That is we do not assign a system to be in thermal equilibrium when ρ_{know} is in line with one of the thermodynamic ensembles. We ask about the macroscopic properties of the system, such as its energy distribution or the temperature, which are akin to X and not to ρ_{know} [128, 174]. The upshot is this: a phase point X is in thermal equilibrium if it displays the macroscopic thermal behavior of the system. Further it is obvious that we are not able to pin down the exact point in phase space. But that does not mean that a probabilistic treatment has to rely on the ignorance of an observer.

The questions we are asking are related to the physical system and not to our knowledge [128]. If we don't know anything about, say a cup of coffee, we should better make a measurement and find, say its temperature. Just come to think of drinking a cup of coffee, where the chance of burning your mouth is 50/50 just because that follows from the indifference principle!

Another aspect of ensemblism is stated by Balian:

"Predictions about macroscopic systems therefore are not deterministic in nature, but rather our best guesses in a statistical sense. Rather than describing a particular system, one treats a *statistical ensemble* of identical systems, all prepared in the given experimental conditions, but differing from one another on the microscopic scale due to the uncertainties arising from the incomplete nature of the preparations. This kind of theoretical approach corresponds to the problem as it occurs in practice: a physical law is established by repeating the same experiment a large number of times and the microscopic variables are not the same for each experiment. Only the probability law for these microscopic variables remains the same for all samples, for given macroscopic conditions. Predictions in physics are thus always statistical in nature, as only macroscopic quantities can be controlled, and as science does not deal with individual objects." [11, p.20]

A few things come to mind here. While the statement of Balian carries a law of large number type argument (and is thus in spirit of typicality) it somehow takes a wrong turn by saying that predictions are "statistical in nature". It seems that the scientific practice of induction is mixed up with the view that ensembles are multiple copies of the same system *at once* and not "after another". Further one can not take care of "individual objects". Well that seems odd. Aren't we interested in whether this specific cup of coffee thermalizes, that is an *individual* system? Another point

⁷Similarly for the quantum realm, but since a wave function ψ is not quite the analog of a phase point, we discuss the classical case here.

is misleading, namely that the evolution is “not deterministic”. Well it is, as the Hamilton equations and the Schrödinger equation clearly are. What should be said is that the typical microscopic trajectories lead to emergent empirical regularities.

Still it is worthwhile to note that there is a way to make sense of the Gibbs ensembles. Not referring to an observer, a view of probability is sometimes called “frequentism” and considered as an “objective” notion of probability (see, .e.g., [34]).

While one has to admit that the Gibbsian view is practical for computations (see, e.g., [188, p.443],[121] and also Part III) and can be viewed as an effective theory [105] it has severe conceptual problems as we’ve just discussed and will discuss throughout this thesis.

First a system does not possess a ρ [136]. Although not accessible in practice via measurements it is hard to doubt that a system is not in an exact micro state X . It is also not clear which ρ to choose a priori. One can argue that by the indifference principle, each outcome is equally likely, but depends on the application! It’s clearly misleading, as pointed out nicely by Ma [188], that when asking how much days in a year it rains in a particular forest in china, then the answer following the indifference principle would be roughly 150 days. Which is wrong. Again one is inferring the micro-canonical distribution, by following the indifference principle. But that is not answering the question why systems are in thermal equilibrium. It answers the question, which probability distribution is the correct one in thermal equilibrium by positing what is already known by experiment.

Second, whether a system has a certain state or not does not rely on our knowledge. A view not shared by ensemblist: “the idea of the precise state of a system is in any case an abstract limiting concept.”([281], p. 1). We disagree in the sense that we think it’s reasonable to say that there is a specific state a system has, even if we do not have access to it⁸. Put briefly: we do not know, but nature knows what state it is in.

What comes to mind is a famous quote from Schrödinger, which he stated in context of the measurement problem, but it also fits in nicely in the critique of the ensemblist discussion:

“There is a difference between a shaky or out-of-focus photograph and a snapshot of clouds and fog banks”[240].

In the ensemblist view the clouds refer to a probability density expressing degrees of belief. Of course we have a too coarse view on many particle systems. But instead of treating this pragmatically, the ensemblist treats fog banks as fundamental. We now elaborate individualism, where thermal properties are actual properties of a system. Although the fog banks might not go away completely, it is believed that there’s something behind them.

⁸Such a view might be coined “scientific realism”, which is hard to “prove” [47].

The key elements of **individualism** are rather simple and natural. An individual system is a single system. Examples are a cup of coffee⁹ or a thermos bottle [128, p.3]. And as already mentioned the question one is asking is this: what does it *mean* for a system to be in thermal equilibrium? Why is a system in thermal equilibrium? Let us dwell on the classical case for a moment. From an individualist perspective a system does not have a ρ , but an *actual* state described by the momenta and the positions of all the particles, that is a single point X in phase space Γ . Of course, we do not know the exact state X , but that is not relevant for the system being in thermal equilibrium. It's not whether an observer knows the exact state, but whether *nature knows*, that is there is an *actual* state independent of an observer. In principle nothing speaks against nature being fundamentally random. What is problematic in the discussion so far is that randomness is understood in terms of the ignorance of an observer¹⁰. What's relevant is whether the energy is spatially distributed in a system in such a way that the temperature is locally constant and the same everywhere in the system. For such a system it also follows that other macro variables (besides energy) have roughly constant values. As a consequence of reductionism a micro state should also represent these macro states. The relevant set of phase space is given by $\Gamma_E = \{X : H(X) = E\}$, where H is the Hamilton function, i.e., Γ_E consists of points with the same energy. Depending on the macro variables chosen one can partition Γ_E into regions Γ_ν , i.e., $\Gamma_E = \bigcup_\nu \Gamma_\nu$, such that different micro states in each Γ_ν macroscopically give the same look. Among those Γ_ν is the thermal equilibrium state Γ_{eq} , which occupies almost the entire energy surface $\text{vol}(\Gamma_{\text{eq}}) \approx \text{vol}(\Gamma_E)$ (here vol denotes volume or size or measure). That means almost any $X \in \Gamma_E$ represents thermal equilibrium. That is from an individual perspective the essence of thermal equilibrium: most micro states are such that they look macroscopically as if they are in thermal equilibrium. And that is just a fact and not related to the knowledge we have about the particular micro state.

Now in quantum mechanics things are a little bit more subtle as density matrices do not only arise due to a lack of knowledge¹¹, but also as reduced density matrices, i.e., from entanglement. That means for a system in a pure state, the reduced density matrix can be a mixed state. We discuss this in more detail below.

Nevertheless, the analog in quantum mechanics (although not quite correct, see [136, p.12]) of a phase point X in classical mechanics is a pure state, that is a wave function $\psi \in \mathbb{S}(\mathcal{H})$ (well not precisely, as the analog would be (Q, ψ) with Q the particle configuration, see Section 3.3.2). Although a system does not necessarily have to be in a pure state, one can still properly define what it means for a wave function $\psi \in \mathbb{S}(\mathcal{H})$ to be in thermal equilibrium. It even turns out that there

⁹Leaving subtleties of this not being a closed system to the side for the sake of the discussion here.

¹⁰Notice already the similarity to quantum mechanics and the measurement problem.

¹¹Further lack of knowledge can really mean limitations to knowledge in the sense that there is a fundamental epistemic barrier, see [287].

are two notions: macroscopic thermal equilibrium (MATE) and microscopic thermal equilibrium (MITE)[127, 128](see below). Similar in spirit, but more involved due to macro variables being self-adjoint operators and thus not commuting in general one can still argue that there is a decomposition of $\mathcal{H}$ into subspaces

$$\mathcal{H} = \bigoplus_{\nu} \mathcal{H}_{\nu} \quad (1.7)$$

with projector $\hat{P}_{\nu}$ and dimension $\dim \mathcal{H}_{\nu}$ (we will see this in Chapter 2). Among those subspaces, to which a macro state ν is associated, is one corresponding to thermal equilibrium, which has by far the largest dimension $d_{\text{eq}}/D \approx 1$. A system is in MATE, if ψ is arbitrarily close to the thermal equilibrium subspace $\mathcal{H}_{\text{eq}}$. Let $\hat{P}_{\text{eq}}$ be the projector onto $\mathcal{H}_{\text{eq}}$, then for $\psi \in \mathbb{S}(\mathcal{H})$ being in MATE means that

$$\langle \psi | \hat{P}_{\text{eq}} | \psi \rangle \approx 1. \quad (1.8)$$

That is one can make sense of thermal equilibrium also considering pure states and not mixed states. Having this in mind let us now discuss a key problem of statistical physics.

1.2. The Problem of Irreversibility

The problem of irreversibility arises as a conflict between two levels of description. Macroscopic systems have the tendency to move towards a stationary state and stay there for a sufficiently long time. That is their dynamics is irreversible in time. This has been famously coined by Clausius in the second law of thermodynamics, which makes use of a special physical quantity, called heat, which has an astonishing property:

”Die Wärme hat die Eigenschaft, unter gewissen Umständen mit gewöhnlicher mechanischer Arbeit vergleichbar zu sein, und geht ferner, wenn zwei Körper von verschiedener Temperatur sich berühren, immer vom wärmeren zum kälteren über, aber nie umgekehrt.”¹²

The two laws of thermodynamics in the words of Rudolf Clausius referring not only to subsystems, but to the world as such¹³

¹²[42, p.356], and can be translated roughly as

”Heat has the property under given circumstances to be comparable with ordinary mechanical work and if two bodies which are at different temperatures are put together then the heat always flows from the hotter to the colder one and never in the other direction.”

¹³Cf. [69, p.400]. English translation:

1) The energy of the world is constant.

- 1) Die Energie der Welt is constant.
- 2) Die Entropie der Welt strebt einem Maximum zu.

While macroscopic systems ultimately consist of particles following certain laws of motion, these should also inherit such a behavior. For either classical or quantum mechanics, this is not the case. The equations of motion stay invariant under time reversal: consider closed macroscopic quantum system $\mathcal{S}$ with Hilbert space $\mathcal{H}$ and micro state $\psi \in \mathbb{S}(\mathcal{H})$ evolving unitarily according to (1.2). If ψ_t is a solution of (1.2), then also ψ_{-t}^* is a solution of (1.2). Thus the dynamics is invariant under time reversal. By reductionism this leads to the

Problem of Irreversibility: Why do systems show macroscopic irreversible behavior, while the underlying microscopic dynamics is reversible? In other words: why do systems evolve into equilibrium?

Of course, several proposals on the problem of irreversibility have been made. Some of them trying to change the underlying dynamics [9, 57]. For instance by claiming that the microscopic theory, being Schrödinger quantum mechanics or Hamiltonian mechanics is not correct, and one has to “go deeper” to particle physics and take the CPT theorem into account (see [9] and the cited references). Another proposal is that the collapse of the wave function is decisive to the problem of irreversibility [1]. That however would mean that resolving the problem relies on an observer or a measurement. Another common claim is that systems in reality are never isolated and thus one has to focus on the dynamics of an open system (e.g. a Lindblad equation). While that is certainly correct, it still might be interesting to see whether entropy increases in a closed system. Besides that, recent experiments try to do so (see [273] and the cited references therein). A view however that comes to an end when considering the whole universe¹⁴. Note that Clausius formulation of the second law points exactly at that: the entropy of the universe strives towards a maximum. Another proposal is to appeal to chaotic systems, which also have a certain special dynamics and are related to the eigenstate thermalization hypothesis (see, e.g., [9, 31, 74]).

We do not take the just stated considerations into account here. The conflict stated above is well posed. For classical systems it has been resolved by Boltzmann in his infamous works on the Boltzmann equation and the H-theorem [27, 28]. In this thesis we focus on Boltzmann’s view. It can be extended to quantum systems, also allowing to resolve the conflict. This is pointed out in Part II. For further

2) The entropy of the world strives towards a maximum.

¹⁴ Although recently the question was raised in what sense the universe can be considered as an open system, see e.g. [231], p.11 or [70] and references therein.

analysis of Boltzmann's contribution and the discussion of some misconceptions often encountered among physicists and philosophers of science see [9, 170, 169].

In similar spirit quantum mechanically, a wave function ψ_t evolves unitarily through Hilbert space until it reaches and stays close to $\mathcal{H}_{\text{eq}}$ for most of the time. Also here Poincare recurrence has to be taken into account.

Regarding thermalization of closed quantum systems from an **individualistic** perspective different notions are used, in particular with respect to MATE. Let $\hat{P}_{\text{eq}}$ denote the projector onto the thermal equilibrium subspace $\mathcal{H}_{\text{eq}}$. That means a pure state $\psi_0 \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ thermalizes if

$$\langle \psi_t | \hat{P}_{\text{eq}} | \psi_t \rangle \approx 1 \quad (1.9)$$

for most of the time t . There are several works in spirit of this [272, 127, 128, 130, 123, 125]. Quite general the idea is as follows: a system with initial pure state $\psi_0 \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ thermalizes relative to a set of suitable observables $\mathcal{A}$ if for all $\hat{A} \in \mathcal{A}$

$$\langle \psi_t | \hat{A} | \psi_t \rangle \approx \text{tr}(\hat{\rho}_{\text{mc}} \hat{A}) \quad (1.10)$$

for most times t .

The **ensemblistic** view has a mathematically well posed meaning for thermalization [7], that is

$$\hat{\rho}_t \rightarrow \hat{\rho}_{\text{can}} \quad (1.11)$$

as $t \rightarrow \infty$. However, here we focus on different breeds related to observables: a system in an initial state $\hat{\rho}_0$ thermalizes relative to a suitable set $\mathcal{A}$ if for all $\hat{A} \in \mathcal{A}$ it equilibrates and further $\hat{\rho}_{\text{eq}} = \hat{\rho}_{\text{mc}}$, more precisely

$$\text{tr}(\hat{\rho}_t \hat{A}) \approx \text{tr}(\hat{\rho}_{\text{mc}} \hat{A}) \quad (1.12)$$

for most times t . This is also known as thermalization on average as opposed to thermalization during time intervals (see [116] and references therein).

Remark 1.2.1 (Ergodicity). Let us briefly mention a common approach taken in thermalization of systems, that is ergodicity (see, e.g., [211, 26, 29, 292, 161]). It has ensemblistic and individualist aspects. The reason we mention it at this point has several reasons: first, it turns out that it is neither necessary nor sufficient for thermalization and second a quantum analog will be discussed later (see, e.g., [119, 284]). A further reason is actually a conceptual one regarding criticism of the typicality approach. The ergodic hypothesis leads to unnecessary rigor in explaining thermalization [169, Ch. 9]. Actually showing that a system is ergodic can only be done for certain simplified cases (see, e.g., [253, 38, 252]). However, it is believed that realistic systems are ergodic. A last point is that it is used to justify the micro-canonical measure or the micro-canonical density matrix in quantum mechanics (see also Part III). Ergodicity

is also used regarding thermalization in quantum systems and has first been worked out by von Neumann [297] (for a more general discussion see [151]). $\diamond$

1.3. Status of Ensembles for Subsystems

Ensembles are extremely useful in equilibrium thermodynamics. However, their justification is still up to debate. It is a fundamental question of statistical mechanics to find such a justification [212, p.1940],[121, 136]. As a system does “not have” a ρ or a $\hat{\rho}$, but an actual state X or ψ (one has to be a bit cautious with quantum mechanics here, see [136]) and one should think of ensembles, as Schrödinger put it, as “mental copies of the one system under consideration”[241, p.3] and a pragmatic tool for computations, but not as fundamental.

Consider a closed system, say a box, confined to some region in space $\Lambda \subset \mathbb{R}^3$ with finite volume $\text{vol}(\Lambda) = V$. Let $S \subset \Lambda$ be a subsystem S and a heat bath $B = \Lambda \setminus S$, such that $S \cup B$ is the total system. In the standard cases, S and B can exchange energy or particles¹⁵, which lead to either the canonical $\hat{\rho}_{\text{can}}$ or the grand-canonical ensemble $\hat{\rho}_{\text{gc}}$. Depending on the particular interest one can choose the appropriate ensemble in order to compute relevant properties (an instance of equivalence of ensembles [34]). Both $\hat{\rho}_{\text{can}}$ and $\hat{\rho}_{\text{gc}}$ are derived from the micro-canonical density matrix $\hat{\rho}_{\text{mc}}$ defined on the Hilbert space of $S \cup B$, by tracing out the bath degrees of freedom.

These ensembles provide a powerful machinery to compute thermodynamic quantities. Let us consider for instance the canonical ensemble

$$\hat{\rho}_{\text{can}} = \frac{1}{Z} e^{-\beta \hat{H}}, \quad (1.13)$$

where $\beta = 1/k_{\text{B}}T$ is the inverse temperature, $\hat{H}$ the Hamiltonian and Z the canonical partition function. With $\hat{\rho}_{\text{can}}$ one can compute the energy E of the macroscopic system via

$$E = \text{tr}(\hat{\rho}_{\text{can}} \hat{H}). \quad (1.14)$$

Further, what seems “only” as a normalization constant is connected to the free energy F of the system, namely

$$F = -\beta^{-1} \log Z. \quad (1.15)$$

As the free energy is the naturally associated thermodynamic potential of the canonical ensemble one can compute other quantities, such as pressure etc. from it via standard thermodynamic computations. Similar considerations can be done for the other standard ensembles [11, p.220].

As mentioned the micro-canonical density matrix $\hat{\rho}_{\text{mc}}$ is used to derive the other

¹⁵For more on this see Part III.

ensembles by fairly standard, conceptually unproblematic, methods. That is in order to justify the use of ensembles one has to explain why $\hat{\rho}_{\text{mc}}$ appears. More explicit, why for a closed system $S \cup B$, the state in thermal equilibrium is given by $\hat{\rho}_{\text{mc}}$. As we will argue this is the case, because it is typical. Most pure states on the energy shell of the total system $S \cup B$ are such that it appears to have density matrix $\hat{\rho}_{\text{mc}}$. This is in stark contrast to other proposals in the literature justifying the use of $\hat{\rho}_{\text{mc}}$ (for more details see Part III), by appealing to either the so called “principle of equal a priori probabilities” or the maximum entropy principle. As the latter can be seen as an extension of the former let us just say that given the von Neumann entropy one maximizes it under the constraint that the total energy is fixed. This leads directly to $\hat{\rho}_{\text{mc}}$. Akin to this approach is the knowledge an observer has about a system. A problematic notion as we shall show in Part III.

The discussion on the status of ensembles goes beyond physics as it includes philosophical considerations, such as the epistemological role of an observer and the very meaning of probabilistic reasoning in physics and in general. Cleaning up these issues goes far beyond the scope of this thesis. Still we have a particular point of view, which briefly stated is this: physics does not depend on the knowledge of an observer. Not classical physics and also not quantum physics. There are facts in nature, which happen independently of a measurement or the knowledge of an observer. For example, we will argue that for most wave functions on an appropriate subset of the total Hilbert space of $S \cup B$, a system S in thermal equilibrium appears as if it were in a state given by the appropriate (canonical) density matrix. That is in our view [136, 175] the status of ensembles is best understood in terms of typicality. In particular, there is no need for repetition or sampling procedures, as would be required when ensembles are interpreted from a frequentist perspective.

We now discuss individualistic notions of thermal equilibrium for S , that do not rely on subjective knowledge about a system. Let us start with the description of S in terms of reduced density matrices. Consider as above a setup of subsystem S and heat bath B with respective Hilbert spaces $\mathcal{H}^S$ and $\mathcal{H}^B$, such that $S \cup B$ has Hilbert space $\mathcal{H} = \mathcal{H}^S \otimes \mathcal{H}^B$. There is a clear definition what it means for a pure state $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ with $\mathcal{H}_{\text{mc}} \subset \mathcal{H}$ to be in microscopic thermal equilibrium (MITE), namely that

$$\text{tr}^B |\psi\rangle\langle\psi| = \hat{\rho}_{\psi}^S \approx \hat{\rho}_{\text{mc}}^S, \quad (1.16)$$

where $\hat{\rho}_{\text{mc}}^S$ is the micro-canonical density matrix of S . MITE is (as its name says) a more microscopic notion of thermal equilibrium than MATE. Not only that: it is based on a purely quantum phenomena, namely entanglement. It is a seminal result [133], that most $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ (where “most” is understood such that ψ is chosen uniformly from $\mathbb{S}(\mathcal{H}_{\text{mc}})$), are such that

$$\text{tr}^B |\psi\rangle\langle\psi| \approx \text{tr}^B \hat{\rho}_{\text{mc}} = \hat{\rho}_{\text{mc}}^S \quad (1.17)$$

for B large enough.

Further we say that $\psi_0 \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ thermalizes relative to a suitable class of observables, for instance given by operators acting on S and trivially on B , of the form $\hat{A} = \hat{A}^S \otimes \hat{I}^B$ if

$$\text{tr}(\hat{\rho}_{\psi_t}^S \hat{A}^S) \approx \text{tr}(\hat{\rho}_{\text{mc}}^S \hat{A}^S) \quad (1.18)$$

for most times. Recent works in that spirit are [228, 269, 226, 227, 85, 22, 155, 117, 12]; see also [202, 116] for a general overview.

Let us just briefly state another way to talk reasonably about the objective fact of systems being in thermal equilibrium. One can assign a wave function $\psi^S \in \mathbb{S}(\mathcal{H}^S)$ to S , called the conditional wave function. And it can be shown [134, 132] that for typical systems with large enough B , there is a universal thermal equilibrium distribution μ_{eq} on $\mathbb{S}(\mathcal{H}^S)$ of ψ^S , i.e.,

$$\psi^S \sim \mu_{\text{eq}}. \quad (1.19)$$

As these distributions appear from a typicality analysis they do not rely on any subjective knowledge and can be considered as the thermal distributions that appear in nature (for details see Part III and Appendix 11.2). Let us elaborate a bit more on that. Density matrices arise as statistical operators for wave functions ψ that are sampled according to some probability measure μ . That is for $\psi \sim \mu$ the density matrix (“statistical mixture”) reads

$$\hat{\rho}_\mu = \mathbb{E}|\psi\rangle\langle\psi|, \quad (1.20)$$

where $\mathbb{E}$ is the expectation value with respect to μ . It will be shown below in Part III that here is a particular thermal equilibrium measure, called the GAP measure. For each density matrix $\hat{\rho}$ one can assign a $\text{GAP}_{\hat{\rho}}$ measure to it. In particular for thermal equilibrium. As mentioned, the $\text{GAP}_{\hat{\rho}}$ are universal or the typical measures. From that point of view ensembles (in thermal equilibrium) mean the following. A point on $\mathbb{S}(\mathcal{H}^S)$ looks like $\text{GAP}_{\hat{\rho}}$ -most points on $\mathbb{S}(\mathcal{H}^S)$.

2. Boltzmannian Quantum Framework

We now introduce the key concepts of the Boltzmannian quantum framework (BQF). As elaborated above the micro state of a closed macroscopic quantum system is given by a wave function $\psi \in \mathbb{S}(\mathcal{H})$. In Section 2.1 we explain how wave functions are related to macroscopic states. In Section 2.2 we sketch the dominance of thermal equilibrium. Afterwards in Section 2.3 how typicality arguments are used to make statements about whether a system is in thermal equilibrium (with a particular emphasis on random Hamiltonians). Then in Section 2.4 we discuss what it means for wave functions to lie in thermal equilibrium and in Section 2.5 how they get there and which states they reach. Results that discuss the time it takes to reach equilibrium are given in Section 2.6. We end with Section 2.7 by comparing the quantum with the classical case. Throughout this Chapter we use the notation $[K] = \{1, \dots, K\}$.

2.1. Coarse-Graining: Macro Spaces

Let us begin with the notion of a macro space; we follow [9, 128, 284]. In quantum mechanics **macro observables** are given by self adjoint operators $\hat{M}_1, \dots, \hat{M}_K$ (or more general by POVMs) on a Hilbert space $\mathcal{H}$. These can arise as follows: let $\mathcal{S}$ be a closed macroscopic quantum system, say a box $\Lambda \subset \mathbb{R}^3$, with finite volume $\text{vol}(\Lambda) = V$. Suppose that Λ is partitioned into regions/cells Λ_i small on the macroscopic level, but large enough microscopically to contain sufficiently many degrees of freedom. Then a macro observable could for instance be the number of particles in each cell, or the energy per cell or the magnetization per cell.

Each macroscopic observable $\hat{M}_i$ will be suitably **coarse-grained**. The eigenvalues of $\hat{M}_i$ are separated by gaps $\Delta \hat{M}_i > 0$ that are as large as the imprecision of the measurement device. That is, on a macroscopic level, many eigenvalues give the “same look”. The spectrum of the coarse-grained $\hat{M}_i$ reads $\{k \in \mathbb{Z} : k \Delta \hat{M}_i\}$, which means that each eigenvalue is highly degenerate.

A coarse-graining procedure can for instance look like this: for each $i \in [K]$

$$g(\hat{M}_i) = \left\lceil \frac{\hat{M}_i}{\Delta \hat{M}_i} \right\rceil \Delta \hat{M}_i, \quad (2.1)$$

where $\lceil x \rceil$ yields the nearest integer to $x \in \mathbb{R}$; that is (2.1) is for each i a step function. Instead of considering the list of coarse-grained macro variables according to (2.1),

2. Boltzmannian Quantum Framework

we simply denote also the coarse-grained macro variables as $\hat{M}_1, \dots, \hat{M}_K$. The energy is among those macro variables, which means that the neighbouring eigenvalues of $\hat{H}$ are smaller than the macroscopic resolution ΔE , this leads to $\hat{M}_1 = g(\hat{H})$ with $g(x)$ as in (2.1). The coarse-grained spectral decomposition now reads

$$g(\hat{H}) = \sum_n g(E_n) |\phi_n\rangle \langle \phi_n|. \quad (2.2)$$

Since these are operators on $\mathcal{H}$ they do not commute in general. In addition to the coarse-graining procedure, von Neumann argued, one can approximate them by “rounded” operators $\hat{M}'_i$, which do commute¹⁶. More explicitly, say that $\hat{M}_i \approx \hat{M}'_i$, such that

$$[\hat{M}'_i, \hat{M}'_j] = 0 \quad \text{with} \quad i \neq j. \quad (2.3)$$

Then finally following von Neumann [297] (and also Einstein [88]), one can decompose the energy shell¹⁷ into mutually orthogonal subspaces $\mathcal{H}_\nu$,

$$\mathcal{H}_{\text{mc}} = \bigoplus_{\nu} \mathcal{H}_\nu, \quad (2.4)$$

where $\nu = (\nu_1, \dots, \nu_K)$. Each $\mathcal{H}_\nu$ is defined as the joint eigenspace of the $\hat{M}_i$ with eigenvalue m_i , more explicit

$$\mathcal{H}_\nu = \bigcap_{i=1}^K \mathcal{H}_{\hat{M}_i, m_i}. \quad (2.5)$$

Each $\mathcal{H}_\nu$ is associated with a **macro state** ν with dimension $\dim \mathcal{H}_\nu = d_\nu$ and respective projector $\hat{P}_\nu$.

The argument of von Neumann that operators can be approximated such that their approximations commute has raised the question whether that is mathematically possible. In other words: given $\hat{M}_1, \dots, \hat{M}_K$, can we find commuting operators $\tilde{M}_1, \dots, \tilde{M}_K$ that approximate $\hat{M}_1, \dots, \hat{M}_K$. For $K = 2$ it does work [179] and for $K = 3$ it does in general not work [145]. Further Ogata [207] has shown that for certain average quantities in quantum spin systems there are exactly commuting operator approximations.

Practically $\hat{M}_1, \dots, \hat{M}_K$ do not commute in general, but still the arguments of von Neumann are reasonable to proceed and we will do so here, i.e., from now on we will consider (2.4) as given. Nevertheless there are also approaches not relying on a collection of “rounded” operators [221, 272, 75].

¹⁶Observables, as being macroscopic, can be measured simultaneously [211, p.20], and relate to a hydrodynamic and thermodynamic description [9, Sec. 5.2.4].

¹⁷Where we restricted the values of all the other $\hat{M}_i$'s besides $\hat{M}_1 = \hat{H}$ to the energy shell $\mathcal{H}_{\text{mc}}$.

2.2. Dominance of Thermal Equilibrium

For each energy shell $\mathcal{H}_{\text{mc}}$ with $\dim \mathcal{H}_{\text{mc}} = d_{\text{mc}}$, there is a subspace $\mathcal{H}_{\text{eq}}$ corresponding to thermal equilibrium, which has by far the largest dimension. More precisely,

$$\frac{d_{\text{eq}}}{d_{\text{mc}}} = 1 - \varepsilon, \quad (2.6)$$

with $0 < \varepsilon \ll 1$.

Dominance of thermal equilibrium implies that macro observables $\hat{M}_i$ are almost constant on $\mathcal{H}_{\text{mc}}$, meaning that the respective eigenvalue has degeneracy of at least $d_{\text{eq}} \approx d_{\text{mc}}$.

It is expected to be true in general and can be shown in many cases (see e.g. [131, 130, 128]) that $\mathcal{H}_{\text{eq}}$ exists. For instance one can argue that ε is exponentially small in the number of particles in the following way (although the reasoning is classically, it also applies to the quantum realm): let $\Lambda \subset \mathbb{R}^3$ containing N particles and partition it into m cells Λ_i (all of equal volume), which are small on the macroscopic scale, but microscopically large enough to contain sufficiently many degrees of freedom. Now let $\hat{M}_j = \lceil (N_j/N) \Delta \hat{M}_j \rceil \Delta \hat{M}_j$, where N_j denotes the number of particles in each cell Λ_j and resolution $\Delta \hat{M}_j > 0$. For reasonable choices of m and $\Delta \hat{M}_j$ one can argue that

$$\varepsilon = \exp(-10^{-15} N). \quad (2.7)$$

Further it is well known empirically that such a dominant state exists. Still it remains hard to prove that it's instantiated for a concrete microscopic $\hat{H}$ [9, p.78]. However there are examples, say a box divided into two parts, where one can argue that in such a case for suitably chosen macro variables (e.g. energy distribution or particle number; and thus any extensive macro variable) a dominant subspace $\mathcal{H}_{\text{eq}}$ is expected to exist [130]. On the other hand there are also counterexamples [127].

2.3. Typicality in QSM

Typicality reasoning is used vitally in quantum statistical mechanics (QSM) and here we state some of its common arguments (for a general discussion of the concept of typicality see Section 3.1). Thermal equilibrium (and related notions) emerges mainly due to concentration of measure phenomena making use of the high dimensions of Hilbert spaces.

Typicality Measures in QSM

Let $\hat{A}$ be a self-adjoint operator and $\hat{\rho}$ a density matrix on a finite-dimensional Hilbert space $\mathcal{H}$ with dimension $\dim \mathcal{H} = D$. In QSM one is usually interested in the

2. Boltzmannian Quantum Framework

behavior of quantities such as (see [72] and [202, 116] for a more general overview of typicality results)

$$\mathrm{tr}(\hat{A}\hat{\rho}_t) = \sum_{n,m} e^{it(E_n - E_m)} \hat{\rho}_{mn}(0) \hat{A}_{nm}, \quad (2.8)$$

where $\hat{\rho}_{mn}(0) = \langle \phi_m | \hat{\rho} | \phi_n \rangle$ and $\hat{A}_{nm} = \langle \phi_n | \hat{A} | \phi_m \rangle$; although put in an ensemblistic style, one can also simply consider pure states only. Now typicality statements refer to how “most” $\mathrm{tr}(\hat{A}\hat{\rho}_t)$ behave. To do so one needs to define what “most” means.

Here we will collect some of the common notions of “most” used in the BQF (see, e.g., [133, 131, 130, 134]), but also in other considerations regarding QSM (see, e.g., [183, 218, 222, 272, 214, 143, 109] or [202, 116]). These include states, times, orthonormal bases, decompositions of subspaces and unitary matrices. We will discuss Hamiltonians separately as they play a central role in Part II. Roughly said the discussion boils down to probability measures on the unit sphere and the uniform measure on the unitary group.

Before we start let us emphasize that choosing wave functions, Hamiltonians and so on according to some probability measure $\mathbb{P}$ does *not* mean that these are *inherently* random (see, e.g., [9, 221, 222, 272]). It further does not mean that repeating certain experiments, say for a given $\hat{H}$, yields a distribution close to $\mathbb{P}$. However, typicality statements exclude certain “bad” cases. Once a behavior is shown to be typical and we also expect it to be typical, there is nothing left to explain (unless we have good reasons against it), a point further explored below in Section 3.1.

We begin with states. Let $\varepsilon > 0$ and let $\mathbb{P}$ be a probability measure on $\mathbb{S}(\mathcal{H})$. Then a statement $s(\psi)$ about $\psi \in \mathbb{S}(\mathcal{H})$ is true for $(1 - \varepsilon)$ -most $\psi \in \mathbb{S}(\mathcal{H})$ if

$$\mathbb{P}\{\psi \in \mathbb{S}(\mathcal{H}) : s(\psi) \text{ holds}\} \geq 1 - \varepsilon. \quad (2.9)$$

For simplicity we sometimes just say “most” (with respect to a certain measure, usually clear from the context) $\psi \in \mathbb{S}(\mathcal{H})$ without taking an ε into account. We also write $\forall \psi$, when we mean “for most ψ ” and similarly for other quantities.

The normalized surface area measure on the unit sphere $\mathbb{S}(\mathcal{H})$ is denoted as $u_{\mathbb{S}(\mathcal{H})}$. It has been introduced by Schrödinger [239, 241], while later worked out more peculiarly by Bloch [9]. It is invariant under the Schrödinger evolution, i.e., it is stationary and thus serves as a natural measure. It is the classical pendant of the Liouville measure. Further it is related to the micro-canonical density matrix in the following way, suppose $\psi \sim u_{\mathbb{S}(\mathcal{H})}$ ¹⁸, then the corresponding density matrix reads

$$\hat{\rho}_{u_{\mathbb{S}(\mathcal{H})}} = \int_{\mathbb{S}(\mathcal{H})} u(d\psi) |\psi\rangle\langle\psi|. \quad (2.10)$$

¹⁸For a random variable X with probability measure $\mathbb{P}$, we write $X \sim \mathbb{P}$.

The normalized area measure provides useful insights to standard quantum mechanical results (see Section 11.1). The uniform measure turns out to be a special case of the so called GAP measures, which we will discuss in Part III.

Let us briefly mention some useful results regarding uniformly distributed vectors on the unit sphere [284, 277]:

Lemma 2.3.1. *Let $\mathcal{H}$ with $D = \dim \mathcal{H} < \infty$, $\psi \sim u_{\mathbb{S}(\mathcal{H})}$ and $\hat{B} : \mathcal{H} \rightarrow \mathcal{H}$:*

$$\mathbb{E}\langle\psi|\hat{B}|\psi\rangle = \frac{\text{tr } \hat{B}}{D}, \quad (2.11)$$

$$\text{Var}\langle\psi|\hat{B}|\psi\rangle = \frac{1}{D(D+1)} \left(\text{tr}(\hat{B}^\dagger \hat{B}) - \frac{|\text{tr } \hat{B}|^2}{D} \right). \quad (2.12)$$

Further, let $\{|\phi_m\rangle\}$ be an ONB of $\mathcal{H}$ and $c_m = \langle\phi_m|\psi\rangle$:

$$\mathbb{E}(c_k^* c_l c_m^* c_n) = 0, \quad \text{if an index occurs only once,} \quad (2.13)$$

$$\mathbb{E}(c_k^{*2} c_l^2) = 0, \quad \text{for } k \neq l, \quad (2.14)$$

$$\mathbb{E}(|c_k|^4) = \frac{2}{D(D+1)}, \quad (2.15)$$

$$\mathbb{E}(|c_k|^2 |c_l|^2) = \frac{1}{D(D+1)}, \quad \text{for } k \neq l. \quad (2.16)$$

Example 1. As a consequence of Lemma 2.3.1 for $\hat{\rho} = |\psi\rangle\langle\psi|$ and $\psi \sim u_{\mathbb{S}(\mathcal{H})}$. [128, 284, 266] one finds

$$\langle\psi|\hat{A}|\psi\rangle = \frac{\text{tr } \hat{A}}{D} = \text{tr}(\hat{\rho}\hat{A}) \quad (2.17)$$

with density matrix $\hat{\rho} = \hat{P}/D$ where $\hat{P}$ is the projector onto $\mathcal{H}$. We will explain the conceptual importance of this result in Part III.

As thermalization refers to a stationary state, the easiest way to get such a state is to average out time. Thus regarding statements about most times, the following notion is used. Here is a definition for "most times" [131, 277]: Let $\delta > 0$. A statement $s(t)$ is said to hold for $(1 - \delta)$ -most $t \in [0, T]$ for $T > 0$ if

$$\frac{1}{T} |\{t \in [0, T] : s(t) \text{ holds}\}| \geq 1 - \delta, \quad (2.18)$$

where $|A|$ is the length of $A \subset \mathbb{R}$. Further $s(t)$ is true for $(1 - \delta)$ -most $t \in [0, \infty)$ if and only if the limes inferior of (2.18) as $T \rightarrow \infty$ is greater or equal to $1 - \delta$ ($s(t)$ typically holds "in the long run.")

The time average is understood as follows: let $f : \mathbb{R}^+ \rightarrow \mathbb{C}$, then the time average

reads

$$\langle f \rangle_T = \frac{1}{T} \int_0^T f(t) dt. \quad (2.19)$$

The infinite time average of f is thus given by $\lim_{T \rightarrow \infty} \langle f \rangle_T$, whenever this limit exists.

In order to make a typicality statement with respect to most times, one can either use Markov's inequality by using the "infinite time limit" or use Chebyshev's inequality (for more details see Section 3.1). For the latter one also has to compute the time variance, which is in general straight forward, but quite involved.

Example 2. As an example consider equilibration [218, 250, 225, 251, 223, 220]. Under certain conditions it is shown that for $(1 - \delta)$ -most $t \in [0, T]$ (2.8) is close to

$$\overline{\text{tr}(\hat{A}\hat{\rho}_t)} = \sum_n \hat{\rho}_{nn}(0) \hat{A}_{nn}. \quad (2.20)$$

Note that δ looks differently depending on the precise setting in the above cited references. Equilibration is different from thermalization as the right hand side of (2.20) is not necessarily the thermal equilibrium value; for more details on equilibration see [116, 202].

Now consider the set $\text{ONB}(\mathcal{H})$ of orthonormal bases of $\mathcal{H}$. On this set the uniform measure $u_{\text{ONB}(\mathcal{H})}$ is defined as follows: choose a vector ϕ_1 , which is uniformly distributed on the unit sphere $\mathbb{S}(\mathcal{H})$. Now let $\mathcal{H}_1$ be the orthogonal complement of ϕ_1 . Now, choose a second vector ϕ_2 uniformly from $\mathbb{S}(\mathcal{H}_1)$. Again let $\mathcal{H}_2$ be the orthogonal complement of ϕ_1 and ϕ_2 and so on and so forth. This leads to a well-defined notion of a uniformly distributed ONB.

Let U be a unitary matrix. Denote the unitary group on a finite-dimensional Hilbert space $\mathcal{H}$ as $\mathcal{U}(\mathcal{H})$. On $\mathcal{U}(\mathcal{H})$ there is a uniform measure called the Haar measure. It is the unique normalized measure that is invariant under multiplication by fixed unitary matrix. There is a natural connection between unitary matrices and ONBs. Let $\{\phi_\alpha\}, \{\chi_\beta\}$ be ONBs. Then there is a (unique) element $U \in \mathcal{U}(\mathcal{H})$ that has matrix representation $U_{\alpha\beta}$ connecting the two ONBs:

$$\phi_\alpha = \sum_\beta U_{\alpha\beta} \chi_\beta. \quad (2.21)$$

That is, the Haar measure on $\mathcal{U}(\mathcal{H})$ induces a probability distribution on the set of ONBs on $\mathcal{H}$. Here one can also see how a uniform distribution of ONBs connects to unitary matrices.

For subspaces we do this. First we fix their respective dimension d . We use the measure on $\text{ONB}(\mathcal{H})$ to get a measure over all d -dimensional subspaces. Now if

$\chi_1, \dots, \chi_D$ is a uniformly distributed ONB, then the random subspace spanned by $\chi_1, \dots, \chi_d$ is considered to be uniformly distributed.

Consider further the family of macro spaces $\{\mathcal{H}_\nu\}$ with fixed number of subspaces and fixed dimension d_ν . Again the measure is defined through the measure on $\text{ONB}(\mathcal{H})$. Consider an ONB $\chi_1, \dots, \chi_D$ and let those χ_α span $\mathcal{H}_\nu$ for which $\alpha \in J_\nu$; here J_ν “carries” all the indices needed to span $\mathcal{H}_\nu$, that is the number of elements in J_ν is d_ν . Or stated differently, the J_ν form a partition of $[D]$.

Typical Hamiltonians as Random Matrices

Random matrices are widely applied in mathematics and physics (see, e.g., [2, 197]). While its development dates back further [256, Sec. 1.1] seminal results of importance for physics are those of von Neumann [297] (a precursor of the eigenstate thermalization hypothesis (ETH) (see [135, Eq.17])) and Wigner [302, 303, 304]. Wigner modelled a system of heavy nuclei by a hermitian random matrix with independent and identically distributed matrix entries. Without carrying about any details (besides hermitian symmetry of the Hamiltonian) of the actual system he obtained the correct energy gap statistics. Such considerations have lead to fruitful research in the past 20 to 30 years as Deutsch [77] in his work on the ETH has used a random Hamiltonian, as well as Srednicki [261] a random matrix ansatz in the context of the ETH. Further mathematical rigorous results have been developed recently in particular by Erdős and collaborators (see the references below). A seminal result is the proof of the ETH for Wigner matrices [63]. This has been extended to Wigner type matrices quite recently in [94] (we will define these matrices below). For further physical applications see [91, Sec. 5][2] and the cited references therein.

We will now explain why random Hamiltonians play such a central role in QSM (see, e.g., [141, 31, 74]) (of closed systems¹⁹); also in this thesis they are of particular interest. That is the case for several conceptual reasons (see, e.g., [232, Sec.2.4] and [9, 130]), which we first discuss and afterwards give examples for random Hamiltonians.

Interactions of many particle systems are described by the Hamiltonian $\hat{H}$. To understand such a system one usually considers a concrete $\hat{H}$, say a standard condensed matter Hamiltonian, or just a rather general form as in (1.3). To show that a system with such a Hamiltonian thermalizes is generically really hard. But there is another way. Instead of considering a particular model one can take a **generic Hamiltonian**. The reasoning behind it goes like this: thermalization is a robust or universal phenomenon. It means that the precise details of the interaction do not matter (so much). Roughly said: a system and its Hamiltonian have to be really special such that they

¹⁹One can show that for a system confined to a bounded region in space the Hamiltonian is given by a matrix.

do not thermalize²⁰. In other words thermalization is typical. That is why one can use a random $\hat{H}$.

Another reason to consider a random $\hat{H}$ is that it might yield a first qualitative understanding, if we have no idea how the exact $\hat{H}$ of a system looks like. If it turns out that a random $\hat{H}$ has a certain property P , we can not surely say that an actual system with its actual Hamiltonian has this property P . But if it turns out that such a P is typical, we have good reasons to believe that most systems behave in such a way and there is no further explanation needed why P happens. Note that $\hat{H}$ being chosen randomly does not mean that its random *per se*.

As a generic Hamiltonian it tries to mimic the physically relevant characteristic of a Hamiltonian, such as few-body and short/long range interactions. This can be done by giving the random matrix a certain variance profile. A central question is which probability measure should be chosen for $\hat{H}$ to take care of the relevant physics. Let us start with the most simple setting and from there move to more complex cases.

But first let us briefly illustrate the idea of this endeavour. Let $\mathbb{P}$ denoted a probability measure on the entries of $\hat{H} \in \text{HM}(\mathcal{H})$, where $\text{HM}(\mathcal{H})$ denotes the set of $D \times D$ hermitian matrices on a Hilbert space $\mathcal{H}$ with dimension $\dim \mathcal{H} = D$. Let $s(\hat{H})$ be a statement about $\hat{H}$. We say that a statement $s(\hat{H})$ about $\hat{H}$ is true for $(1 - \varepsilon)$ -most $\hat{H}$ if

$$\mathbb{P}(\hat{H} \in \text{HM}(\mathcal{H}) : s(\hat{H}) \text{ holds}) \geq 1 - \varepsilon \quad (2.22)$$

with $0 < \varepsilon \ll 1$.

Let us now start with a simple example. Consider a Hamiltonian $\hat{H}$ in spectral decomposition

$$\hat{H} = \sum_n E_n |\phi_n\rangle \langle \phi_n|. \quad (2.23)$$

Let the eigenvalues be fixed and let the ONB of $\hat{H}$ be uniformly distributed according to u_{ONB} ; this allows to prove an ETH [130]. Another possibility is to choose the eigenvalues uniformly distributed among $[E - \Delta E, E]$ as well as the eigenbasis, independently of each other. Let us already mention that it gets more complex, if the eigenvalues and eigenbasis are no longer independent. Closely related matrices are Wigner matrices.

Let $\hat{H} = (h_{ij})$ be a $D \times D$ hermitian matrix, with $i, j \in [D]$. Let $\mathbb{P}$ be a probability measure on entries of $\hat{H} \in \text{HM}(\mathcal{H})$. The characteristics of a random matrix model are then given by

$$\mathbb{E} h_{ij} = 0 \quad \text{and} \quad \mathbb{E} |h_{ij}|^2 = S_{ij} \quad (2.24)$$

with variance matrix S_{ij} (and $\mathbb{E}$ the expectation value with respect to $\mathbb{P}$). There is a

²⁰There are systems that indeed do not thermalize, such as many-body-localized systems [127], but this does not harm our argument here.

huge variety of different random matrix models, mainly differing in the characteristics of the distribution of the entries and of course on the probability measure $\mathbb{P}$. The most simplest ones are Wigner matrices and Gaussian matrices. The latter usually come in three flavours, namely the Gaussian unitary ensemble (GUE), the Gaussian orthogonal ensemble (GOE) and the Gaussian symplectic ensemble (GSE); out of conventional reason we will stick with the term “ensemble” at some places, although we believe it might be better to call them “models”. For Gaussian models, the measure is defined on the entries of $\hat{H}$. The GUE is for instance defined as follows: let $\hat{H} = (h_{ij})$ be a hermitian $D \times D$ -matrix, then for $i < j$: $h_{ij} \sim \mathcal{N}(0, 1/2) + i\mathcal{N}(0, 1/2)$ and $h_{ii} \sim \mathcal{N}(0, 1)$ for all i . Here we use the following notation: the distribution of a random variable X is given by the measure $\Sigma(A) = \mathbb{P}(X \in A)$ and we write $X \sim \Sigma$. Further $\mathcal{N}(\mu, \sigma)$ denotes the Gaussian distribution with mean μ and variance σ (for further details see Section 3.1).

In general one can distinguish two classes [182, p.21]. Random matrix models with independent entries (i.i.d.) and random matrix models with rotational invariance, meaning that the distribution of the entries does not change under the unitary transformation $\hat{H} \rightarrow \hat{U}^* \hat{H} \hat{U}$, where $\hat{U}$ is a unitary matrix [95, 91]. The Gaussian and Wigner matrices lie in the same class of random matrix models.

There are other matrix models, which mimic more realistic physical interactions, than the Wigner matrices or the GUE matrices. These are for instance more generalized versions of Wigner matrices with different variance profile. For example sparse matrices, where most entries are zero. These are known to model few-body interactions [35, 104, 31, 107]. In the same vein banded matrices are of interest (see, e.g., [107, 302, 77, 101, 111, 37, 308, 43, 200], especially [95, Sec. 18.7] and the cited references therein). For such matrices the variance profile has the following structure

$$\mathbb{E}|h_{ij}|^2 = Cg(\kappa|i - j|) \quad (2.25)$$

where C is a positive constant, $g(x)$ is a decaying (symmetric) function, that is for larger i, j the entries (h_{ij}) have smaller variances, than the ones close to the diagonal; while $1/\kappa$ is the band width [107, 95].

We now introduce Wigner matrices (see, e.g., [95, 91]). Let $\hat{H} = (h)_{ij}$ be a $D \times D$ hermitian matrix. The elements h_{ij} are i.i.d. random variables (up to hermitian symmetry $h_{ij} = h_{ji}^*$). Their precise characteristics are defined as follows²¹:

$$\mathbb{E}h_{ij} = 0 \quad \text{and} \quad \mathbb{E}|h_{ij}|^2 = \frac{1}{D}. \quad (2.26)$$

In order to make typicality statements let us denote the distribution of the elements

²¹For further technical assumptions, such as the boundedness of the moments see the cited references in this Section.

of $\hat{H}$ as $\mathbb{P}_{\text{Wig}}$. Physically the Wigner matrix expresses a mean field regime, since each entry h_{ij} is typically of the order $1/\sqrt{D}$. As a consequence this leads to ultrafast thermalization [125, 123, 222]. Roughly said the reason is that the energy in the system is “already” uniformly distributed due to the entries of the matrix having roughly the same size and that there is no spatialness in such a model. That is, the oscillations in the unitary evolution die out rather quickly reaching a stationary value. Another way to say this is that the eigenbasis for such a model is uniformly distributed and thus unrelated to the eigenbasis of an observable (or in our cases the decomposition)(for more details see [277, Sec.3.1]). That is why it would be desirable to consider different matrix models, such as (2.25).

Of key interest is the statistics of the eigenvalues and eigenvectors. It turns out that the resolvent $G(z) = (z - \hat{H})^{-1}$ is the relevant quantity to get there (see Section 7.1).

There are other matrix models beyond the Wigner matrix differing in the characteristics of the distribution and the properties of the variance matrix $\mathbb{E}|h_{ij}|^2$; see [95, 91] for an overview.

Key results regarding thermal properties of many particle systems are the following. Most prominently the proof of the ETH [63, 59, 94], showing thermalization for certain classes of observables evolving according to a Wigner Hamiltonian [65, 92, 265] and the equipartition theorem [61]. This has also lead to more research, see, e.g., [64, 66, 67].

2.4. Macroscopic Thermal Equilibrium (MATE)

In the BQF there are two notions of thermal equilibrium [127, 128]: Macroscopic thermal equilibrium (MATE) and microscopic thermal equilibrium (MITE). We will introduce MATE now. MITE is about thermal equilibrium of small subsystems, which are discussed in Part III.

Thermal equilibrium is a key property of thermodynamic systems. A macroscopic system appears stationary and has a spatially uniform temperature profile. From a microscopic perspective a natural definition for a state $\hat{\rho}$ to represent thermal equilibrium is, whenever $\hat{\rho}$ yields for macroscopic observables those values that are in line with the standard thermodynamic formalism. It turns out that on a microscopic level thermal equilibrium can also be represented by a wave function $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ instead of a mixed state $\hat{\rho}$.

Macroscopic thermal equilibrium (MATE) is defined as follows: a system is in MATE if and only if its state $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ is for $\delta > 0$ an element of

$$\text{MATE}_\delta := \{\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}}) : \langle \psi | \hat{P}_{\text{eq}} | \psi \rangle \geq 1 - \delta\}. \quad (2.27)$$

Such an understanding of thermal equilibrium has also been discussed before in [123, 125, 139, 228, 131, 271], but conceptually worked out first by Goldstein et al. [127,

128].

Note that, if the system's state is given by a density matrix $\hat{\rho}$, then the system is in MATE_δ given

$$\text{tr}(\hat{\rho}\hat{P}_{\text{eq}}) \geq 1 - \delta. \quad (2.28)$$

Now suppose $\psi \in \text{MATE}_\delta$. It follows that for a quantum measurement of $\hat{M}_i$ the value is typically close to the thermal equilibrium value of $\hat{M}_i$. The same is true for a joint measurement of all the $\hat{M}_1, \dots, \hat{M}_K$ [130]. More explicitly, the probability that the eigenvalue of $\hat{M}_i$ is given by its equilibrium value m_{eq} is given by

$$\mathbb{P}(m_i = m_{\text{eq}}) = \langle \psi | \hat{P}_{\text{eq}} | \psi \rangle \approx 1. \quad (2.29)$$

Being in thermal equilibrium is a property that most states inherit, because that is what thermal equilibrium is: typical. This is indeed the case, as most wave functions from the energy shell lie in MATE. Let $\psi \sim u_{\mathbb{S}(\mathcal{H}_{\text{mc}})}$ and let $\hat{P}_{\text{neq}} = 1 - \hat{P}_{\text{eq}}$, then by dominance of thermal equilibrium

$$\frac{\dim \mathcal{H}_{\text{eq}}}{\dim \mathcal{H}_{\text{mc}}} \geq 1 - \varepsilon \quad (2.30)$$

with $0 < \varepsilon \ll \delta$, it follows from Lemma 2.3.1 that

$$u_{\text{mc}}(\text{MATE}_\delta) = u_{\text{mc}} \left\{ \psi \in \mathbb{S}(\mathcal{H}_{\text{mc}}) : \langle \psi | \hat{P}_{\text{neq}} | \psi \rangle \leq \delta \right\} \quad (2.31)$$

$$= 1 - u_{\text{mc}} \left\{ \psi \in \mathbb{S}(\mathcal{H}_{\text{mc}}) : \langle \psi | \hat{P}_{\text{neq}} | \psi \rangle > \delta \right\} \quad (2.32)$$

$$\geq 1 - \frac{\mathbb{E} \langle \psi | \hat{P}_{\text{neq}} | \psi \rangle}{\delta} \geq 1 - \frac{\varepsilon}{\delta} \approx 1. \quad (2.33)$$

In the last line we used Markov's inequality. The upshot is that the set of exceptional wave functions not lying in MATE_δ has measure at most ε/δ .

In a similar spirit one can argue that most eigenstates of $\hat{H}$ are in MATE. More general, take any ONB $\{b_1, \dots, b_{d_{\text{mc}}}\}$ of $\mathcal{H}_{\text{mc}}$, then

$$\frac{1}{d_{\text{mc}}} \sum_{i=1}^{d_{\text{mc}}} \langle b_i | \hat{P}_{\text{eq}} | b_i \rangle = \frac{\text{tr} \hat{P}_{\text{eq}}}{d_{\text{mc}}} \geq 1 - \varepsilon \quad (2.34)$$

and then by the Markov inequality at least $1 - \varepsilon/\delta$ of the elements of the ONB lie in MATE_δ . As noted above also density matrices can represent MATE. For the sake of completeness, we briefly mention here that most mixed states are also contained in MATE [128].

A similar definition of MATE was given by Tasaki [272] without assuming that the coarse grained observables commute (also in a similar direction by [266, 75]).

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Further Tasaki's notion of thermal equilibrium is also related to pure states, hence an individualistic view. In [128, 127] the proposal of Tasaki has been coined TMATE. Let $\hat{M}_1, \dots, \hat{M}_K$ be a collection of macro variables²², i.e. self-adjoint operators, which do not have to commute pairwise on $\mathcal{H}$. A system in state $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ is in TMATE if and only if

$$\langle \psi | \hat{P}_j | \psi \rangle > 1 - \delta \quad \forall j = 1, \dots, K, \quad (2.35)$$

with

$$\hat{P}_j = \mathbb{1}_{[V_j - \Delta \hat{M}_j, V_j + \Delta \hat{M}_j]}(\hat{M}_j) \quad \text{and} \quad V_j = \text{tr}(\hat{\rho}_{\text{mc}} \hat{M}_j), \quad (2.36)$$

where V_j is the equilibrium value of $\hat{M}_j$, $\mathbb{1}_A$ the characteristic function on a set $A \subseteq \mathbb{R}$ and $\hat{P}_j$ is a projection on the space spanned by eigenvectors with eigenvalues lying in $V_j \pm \Delta \hat{M}_j$. The difference between $\hat{P}_i$ and $\hat{P}_j$ is that the corresponding subspaces are not orthogonal. TMATE can be written differently as

$$\text{TMATE}_\delta = \bigcap_{j=1}^K \{ \psi \in \mathbb{S}(\mathcal{H}_{\text{mc}}) : \langle \psi | \hat{P}_j | \psi \rangle > 1 - \delta \}. \quad (2.37)$$

For all practical purposes TMATE is nice, however technically simpler than MATE, while keeping its spirit. Note that most $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ lie in TMATE, given that for every i the range of $\hat{P}_i$ has almost the full dimension of the energy shell. That is, typicality of thermal equilibrium is also appearing in Tasaki's proposal, an aspect that is key in his considerations [272].

2.5. Thermalization and Equilibration in BQF

In this part we explain how a unitarily evolving quantum state moves towards thermal equilibrium within the BQF. Here,

$$\psi_t = e^{-i\hat{H}t} \psi_0 \quad (2.38)$$

with Hamiltonian $\hat{H}$ and initial state ψ_0 . Discussing this within the BQF means that we aim at an *explanation* for thermal behavior by appealing to typicality. That is under certain conditions on $\hat{H}$ and/or ψ_0 most systems evolve such that ψ_t becomes close to thermal equilibrium for most of the time (in the long run). In this part we will discuss such conditions.

Note that aiming for an explanation might lack mathematical rigor in the following sense: ultimately one would like to show that for any $\hat{H}$ and any initial state ψ_0 the

²²The macro variables are denoted similar as above, but that should not lead to confusion here.

system thermalizes. This is not what we are aiming for and this is not something one might aim at in general [169, Ch. 9.2].

There is a unified way to think about thermalization [9]: let $\mathcal{A}$ be a class of observables. Then we say a system thermalizes relative to $\mathcal{A}$ if:

$$\langle \psi_t | \hat{A} | \psi_t \rangle \approx \text{tr}(\hat{\rho}_{\text{mc}} \hat{A}) \quad \forall \hat{A} \in \mathcal{A} \quad \forall t \in [0, T]. \quad (2.39)$$

In the following we will specify classes of $\mathcal{A}$. Further we will elucidate conditions on the relevant quantities involved, such as $\hat{H}$, initial states ψ_0 , $\hat{A}$, etc. and see how these lead to thermalization. An example of a common condition (if not stated otherwise) makes use of Hamiltonians $\hat{H}$ which have non-degenerate eigenvalues, as well as non-degenerate eigenvalue gaps.

To show that (2.39) holds, one has to consider time averages of $\langle \psi_t | \hat{A} | \psi_t \rangle$ and show that these are close to $\text{tr}(\hat{\rho}_{\text{mc}} \hat{A})$. Thus one has to argue that the time variances of $\langle \psi_t | \hat{A} | \psi_t \rangle$ is sufficiently small. Then by virtue of Markov's inequality (2.39) can be shown to hold.

Approach to MATE

We now discuss the approach to thermal equilibrium in the BQF. This can be done in two ways: approach to MATE and approach to MITE. Here we mainly focus on the former, while the latter is treated in Part III.

In the BQF, $\mathcal{A}$ consists only of $\hat{P}_{\text{eq}}$, that is the main goal is to argue that for typical macroscopic quantum systems $\mathcal{S}$,

$$\langle \psi_t | \hat{P}_{\text{eq}} | \psi_t \rangle \approx 1, \quad (2.40)$$

for most times t . A key condition that any initial state $\psi_0 \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ thermalizes is the eigenstate thermalization hypothesis (ETH), which states that every eigenvector of $\hat{H}$ lies in $\text{MATE}_{\varepsilon\delta}$. This can be seen from the following quick computation: let $\psi_0 = \sum_n c_n \phi_n$ and $\psi_t = \sum_n \exp(-itE_n) c_n \phi_n$, then²³

$$\overline{\langle \psi_t | \hat{P}_{\text{eq}} | \psi_t \rangle} = \sum_{m,n} c_n^* c_m \overline{e^{-it(E_n - E_m)}} \langle \phi_n | \hat{P}_{\text{eq}} | \phi_m \rangle \quad (2.41)$$

$$= \sum_n |c_n|^2 \langle \phi_n | \hat{P}_{\text{eq}} | \phi_n \rangle \quad (2.42)$$

$$\geq \sum_n |c_n|^2 (1 - \varepsilon) = 1 - \varepsilon. \quad (2.43)$$

²³Note that $\overline{e^{i(x-x')t}} = \delta_{xx'}$.

Here it is assumed that $\hat{H}$ has non-degenerate energy eigenvalues [131], an assumption that can also be dropped, see [232, Prop. 1].

The MATE-ETH has not been proven in full generality. There are important results assuming that the Hamiltonian can be modelled by a random matrix. For instance in [130] for a Hamiltonian with its eigenbasis being uniformly distributed. Also recent results show that the ETH holds for random Wigner matrix models [63, 94]. The difficulty is that the more the characteristics of these matrix models mimic relevant physical interactions, the less they can be treated analytically (nor even numerically). Recently Tasaki proved the MATE-ETH for a fermion chain with nearest-neighbour interactions [275, 274].

Normal Typicality

We now discuss normal typicality, a result that has been first obtained by von Neumann [297], elaborated more on in [131, 135] and extended recently in [277, 296, 93]. Here we especially emphasize the type of equilibrium that normal typicality yields.

A seminal result on the long-time behavior of macroscopic quantum systems dating back to von Neumann [297] is the quantum ergodic theorem (QET) and the H-theorem. These are not analogs to their classical counterparts and further it turns out that they are actually closely related. The QET has played an influential role in the discussion of foundations of QSM, in particular it has been argued that its the essential mechanism that underlies thermalization (see, e.g., [281, 151, 159, 209]). Further the QET serves as a theoretical argument in support of the ETH [135].

We mostly follow [131], where von Neumann's QET is discussed in more detail. There a stronger version of normal typicality is provided. Further vibrant misunderstandings about von Neumann's argument are cleared out, that had a wide influence in physics [103, 151, 185, 186, 187, 210, 215, 294].

Let us also mention that von Neumann's arguments on the QET are in favor of the individualist approach as it's about the evolution of a pure state. Further they also appeal to typicality reasoning.

The quantum ergodic theorem (QET) is about the long-time behavior of the quantum state $\psi_t = e^{-i\hat{H}t}\psi_0$ of a macroscopic system enclosed in some finite box. Loosely speaking the QET says the following: let $\mathcal{H}$ be a Hilbert space with dimension D , let $\hat{H}$ be a Hamiltonian with non-degenerate eigenvalues and energy gaps. Suppose $\mathcal{H}$ is decomposed into orthogonal subspaces $\mathcal{H}_\nu$, that is

$$\mathcal{H} = \bigoplus_{\nu} \mathcal{H}_\nu. \quad (2.44)$$

If d_ν is large and $D = \sum_{\nu} d_\nu$, then most families $\{\mathcal{H}_\nu\}$ are such that for any initial

state $\psi_0 \in \mathbb{S}(\mathcal{H})$ and any macro state ν :

$$\|\hat{P}_\nu \psi_t\|^2 \approx \frac{d_\nu}{D} \quad (2.45)$$

most of the time in the long run²⁴.

What does for “most families $\{\mathcal{H}_\nu\}$ ”, that is decompositions of $\mathcal{H}$, mean?²⁵ Fix the number of subspaces, say K of them. Partition the set $\{1, \dots, D\}$ into subsets I_ν , which have size d_ν , i.e., $|I_\nu| = d_\nu$. Let $\{|\chi_j\rangle\}_{j=1, \dots, D}$ be an ONB of $\mathcal{H}_{\text{mc}}$ and let this ONB be uniformly distributed. Now let $\mathcal{H}_\nu$ be spanned by the basis vectors corresponding to I_ν , i.e., $\mathcal{H}_\nu = \text{span}\{|\chi_j\rangle : j \in I_\nu\}$. Through this we obtain a random decomposition $\mathcal{D}$. For the Hamiltonian $\hat{H}$ we fix the eigenvalues $E_1, \dots, E_D$ and sample the eigenvectors uniformly.

The QET by von Neumann relies on the assumption that all $d_\nu \ll D$. This excludes a thermal equilibrium subspace. This has to do with the understanding von Neumann had about thermal equilibrium, namely that the state $\psi \in \mathbb{S}(\mathcal{H})$ is in thermal equilibrium if and only if

$$\|\hat{P}_\nu \psi\|^2 \approx \frac{d_\nu}{D} \quad (2.46)$$

for each $\nu \in \mathcal{N}$. That is no dominant thermal equilibrium is needed among the $\mathcal{H}_\nu$. One can make the argument [128, Sec. 9.2] that this has to do with the fact that the macro variables are too fine grained, that is $\Delta \hat{M}_j$ are chosen too small. As a consequence no coarse-grained macro variable has an eigenvalue that corresponds to an eigenspace with 99% of the dimension of $\mathcal{H}$. Goldstein et al. [131] showed that the assumption that all $d_\nu \ll D$ in von Neumanns argument can be fixed.

A caveat of the typicality approach just discussed is that its assumptions are not realistic, as the eigenbasis of Hamiltonian and subspaces are not unrelated. In realistic systems this is not the case. There the basis of $\hat{H}$ and the macro states are related. If this would not be the case, the system would go straight to equilibrium. But in realistic systems, energy needs to be transported through the system.

Recently this issue has been addressed for three cases: one for general Hamiltonians [277], one for random Hamiltonians [279] and one for a more generic random matrix model [93].

In [277] generalized normal typicality has been introduced for a Hamiltonian $\hat{H}$ with possibly degenerate energy gaps (see [277] for more details). It states that for

²⁴That’s the reason the statement of the QET is coined *normal typicality*, [131, 135], since the concept of normality stems from that of a normal number.

²⁵We discussed this already above in Section 2.3 for general cases, but still it’s helpful to see it for a particular case.

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any macro state μ , most $\psi_0 \in \mathbb{S}(\mathcal{H}_\mu)$ evolve such that for most times t and large enough d_μ one finds

$$||\hat{P}_\nu \psi_t||^2 \approx M_{\mu\nu}. \quad (2.47)$$

Note that this statement should be read as an equilibration statement. This means that a stationary state $M_{\mu\nu}$ is reached, which is not necessarily the thermal equilibrium state. In [277] it is called normal equilibrium and is given by

$$M_{\mu\nu} := \frac{1}{d_\mu} \sum_n \langle n | \hat{P}_\mu | n \rangle \langle n | \hat{P}_\nu | n \rangle. \quad (2.48)$$

If $\nu = \text{eq}$, then $M_{\mu\text{eq}} \approx 1$ for every μ , i.e., we have thermalization. The precise result depends on the maximal degeneracy of the energy gaps of and on the maximum degeneracy of $\hat{H}$.

The result can also be stated for operators $\hat{B} : \mathcal{H} \rightarrow \mathcal{H}$. Then most initial states $\psi_0 \in \mathbb{S}(\mathcal{H}_\nu)$ are such that for most times $t \in [0, T]$

$$\langle \psi_t | \hat{B} | \psi_t \rangle \approx M_{\nu\hat{B}} \quad (2.49)$$

for d_ν sufficiently large with

$$M_{\nu\hat{B}} := \frac{1}{d_\nu} \sum_n \langle n | \hat{P}_\nu | n \rangle \langle n | \hat{B} | n \rangle. \quad (2.50)$$

Note that for initial states “already” in thermal equilibrium, one finds (given that the ETH holds)

$$M_{\text{eq}\hat{B}} \approx \frac{\text{tr } \hat{B}}{d_{\text{eq}}} \approx \text{tr}(\hat{\rho}\hat{B}) = M_{\text{mc}\hat{B}} \quad (2.51)$$

where $\hat{\rho} = \hat{P}/D$ with $\hat{P}$ projector onto $\mathcal{H}$, also using dominance of thermal equilibrium, i.e., $d_{\text{eq}} \approx D$.

The fact that generalized normal typicality (2.47) is true does not mean that the relative error is small. This has been shown in [279] for a specific random matrix. Recently [93] showed that in a random matrix model normal typicality holds (for more details on the model see Section 6.3).

As mentioned above normal typicality leads to a new notion of equilibrium, namely normal equilibrium. In similar spirit to MATE in Section 2.4 one can define **normal equilibrium (NE)** as follows:

$$\text{NE} := \left\{ \psi \in \mathbb{S}(\mathcal{H}_{\text{mc}}) : \langle \psi | \hat{P}_\nu | \psi \rangle = \frac{d_\nu}{D} \right\} \quad (2.52)$$

and generalized normal equilibrium (GNE) as

$$\text{GNE} := \left\{ \psi \in \mathbb{S}(\mathcal{H}_{\text{mc}}) : \langle \psi | \hat{P}_\nu | \psi \rangle = M_{\mu\nu} \right\}. \quad (2.53)$$

This means that besides other statements, most $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ are in NE and most $\psi \in \mathbb{S}(\mathcal{H}_\mu)$ lie in GNE. Further the “approach” results above can be interpreted as the approach to NE or GNE.

2.6. Thermalization Time Scales

The considerations above regarding thermalization have not made any statements on how long a system needs to reach $\mathcal{H}_{\text{eq}}$. That is mainly due to the fact that an infinite time average was taken. We now discuss results on thermalization time scales within the BQF [123, 125].

Unsatisfied with the result of Short and Farelly [251] regarding the usefulness with respect to large systems, Goldstein, Hara and Tasaki [123] proved two theorems about thermalization times. One as a “warning” and one as a “hope”. The former states that there will always be a thermal equilibrium subspace $\mathcal{H}_{\text{eq}}$, for which the thermalization time will be overwhelmingly long. The latter states that there can be a thermal equilibrium subspace that is reached by any initial state after a very short time.

In another paper Goldstein, Hara and Tasaki [125, 124] showed that for a typical subspace the equilibration time (at room temperature) is of the order of $10^{-13}s$. They conclude that

“the moderately slow decay observed in reality is *not* a typical property for a random choice of $\mathcal{H}_{\text{neq}}$. It suggests that we have to take into account some essential features of realistic nonequilibrium subspaces in order to fully understand the problem of thermalization in isolated quantum systems.”[125]

In order to make a typicality statement they chose a generic subspace. The group of all unitary transformations is denoted as $\mathcal{U}(\mathcal{H})$ on the total Hilbert space $\mathcal{H}$ with dimension D . For each element U of $\mathcal{U}(\mathcal{H})$ one can write down a normalized state $|\xi^{(n)}\rangle = U|\phi_n\rangle$, for $n \in [d]$. Now assume U is sampled according to the Haar measure. With this one should have the following picture: there is a d -dimensional subspace $\mathcal{H}_{\text{rand}}$ spanned by $\{|\xi^{(n)}\rangle\}$ with $n \in [d]$. The projection is given by

$$\hat{P}_{\text{rand}} = \sum_{n=1}^d |\xi^{(n)}\rangle \langle \xi^{(n)}|. \quad (2.54)$$

As U is chosen according to the Haar measure on $\mathcal{U}(\mathcal{H})$ the subspace $\mathcal{H}_{\text{rand}}$ is spanned by random vectors. This means that $\mathcal{H}_{\text{rand}}$ now models $\mathcal{H}_{\text{neq}}$. The main result of

[125] is this: let $1 \leq d \ll D$. Then with very high probability (close to one),

$$\frac{1}{\tau} \int_0^\tau dt \langle \psi_t | \hat{P}_{\text{rand}} | \psi_t \rangle \leq \frac{\tau_B}{\tau} \quad (2.55)$$

for any $\psi_0 \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ and τ such that $0 < \tau \leq \tau_{\text{max}}$, where

$$\tau_{\text{max}} := \tau_B \min \left\{ \left(\frac{D}{d} \right)^{1/4}, D^{1/6} \right\}. \quad (2.56)$$

This result does not rely on the ETH. The Boltzmann time is denoted as $\tau_B := h/(k_B T)$ with temperature T . At room temperature $T \approx 300K$, we get $\tau_B \approx 10^{-13}s$. Even for $\tau \approx 10^{-6}s$ the right hand side of the bound does not get larger than 10^{-6} . The consequence is that any initial state will reach equilibrium before one micro-second. A similar observation has been made by Reimann [222].

The conclusions drawn from the results in [123, 125] are that reality lies somewhere in between those two extremes. Let us mention that recently Erdős, Henheik and Vogel [93] proposed a more realistic random setting interpolating between those two extremes.

2.7. Boltzmann's Classical Statistical Mechanics

We now compare the BQF with the classical case. Consider N point particles in a box with volume $\Lambda \subset \mathbb{R}^3$. Then the state of the system is given by a point $X(t) \in \Gamma$ with $\Gamma = \mathbb{R}^{3N} \times \Lambda^N$. That is, it is characterized by its position $q(t) = (\mathbf{q}_1(t), \dots, \mathbf{q}_N(t))$ and momenta $p(t) = (\mathbf{p}_1(t), \dots, \mathbf{p}_N(t))$. These can change in time according to Hamiltonian equations. For the i -th particle these are given by

$$\dot{\mathbf{q}}_i(t) = \frac{\partial H}{\partial \mathbf{p}_i}, \quad \dot{\mathbf{p}}_i(t) = -\frac{\partial H}{\partial \mathbf{q}_i}, \quad (2.57)$$

where H is the Hamilton function. Expressed differently the evolution of a phase point is given by the Hamilton vector field $\mathbf{v}^H(X)$ on phase space

$$\dot{X} = \mathbf{v}^H(X). \quad (2.58)$$

A solution to this ODE is provided by a one-parameter group of transformations $\Phi_t^H : \Gamma \rightarrow \Gamma$, called the Hamiltonian flow. The evolution of $X(t)$ is deterministic: for given initial values $(q(t_0), p(t_0))$ at time $t = t_0$ phase space trajectories are also solutions of equation (2.58) and are carried through Γ by the Hamiltonian flow.

By reductionism, micro states represent macro states. Many different micro states can share the same “macroscopic look”. A key idea is that of coarse-graining; we

follow [284, 128, 9].

Let $M_j : \Gamma \rightarrow \mathbb{R}$, with $j \in [K]$, be a family of macro variables. There are practically unavoidable limitations to macro measurements, say we are able to distinct two macroscopic states by the accuracy $\Delta M_j > 0$. This coarse-grains our actual observable M_j to $\{k\Delta M_j : k \in \mathbb{Z}\}$. In other words, there is a coarse-graining function $g(x) = \lceil x/\Delta x \rceil \Delta x$ ($\lceil x \rceil$ is the next nearest integer of $x \in \mathbb{R}$) for each of the M_j ,

$$g(M_j) = \left\lceil \frac{M_j}{\Delta M_j} \right\rceil \Delta M_j. \quad (2.59)$$

Now two distinct micro states $X_1, X_2 \in \Gamma$ have the “same macroscopic look” if for each observable their macroscopic appearance is the same, more precisely: $\forall j \in [K] : M_j(X_1) = M_j(X_2)$. This allows to partition phase space into regions

$$\Gamma_\nu = \{X \in \Gamma : M_j(X) = \nu_j, \forall j \in [K]\}, \quad (2.60)$$

such that

$$\Gamma = \bigcup_{\nu} \Gamma_\nu. \quad (2.61)$$

Each $\nu = (\nu_1, \dots, \nu_K)$ is called a macro state and is associated with its respective Γ_ν . Among these macro variables are for instance angular momentum, the magnetization, or the number of particles; one can also partition the volume of the system into cells and ask what the angular momentum, magnetization or particle number per cell is. Usually energy is one of the macro variables, that is a suitable coarse-grained version $M_1(X) = g(H(X))$ in the sense of (2.59). As energy is conserved the dynamics is restricted to the energy shell

$$\Gamma_{\text{mc}} = \bigcup_{\nu} \Gamma_\nu. \quad (2.62)$$

The notion of a measure on phase space is crucial for understanding the behavior of a system with a large number of particles. For a closed system energy is conserved and thus one considers the micro-canonical measure μ_E on the energy surface $\Gamma_E = \{X \in \Gamma : H(X) = E\}$, defined as

$$\mu_E(A) = \int_A dX \delta(H(X) - E) \quad (2.63)$$

with $A \subseteq \Gamma_E$. As we considered a particular coarse-graining procedure above, this means that one is usually referring to the energy shell and the respective measure on it (see [284, Sec. 5.2] for a detailed discussion). We will not care about these details here, as it does not change the points we want to make here. We think of the micro-canonical measure simply in terms of “measure” or “size”. By the Liouville theorem,

2. Boltzmannian Quantum Framework

which says that the size of sets in phase space does not change under Hamiltonian time evolution, the measure μ_E is stationary. The notion of a stationary measure is indispensable for typicality reasoning as typical behavior should not depend on time.

Before we state the second law, bear in mind, that among the regions in phase space there is one particular region Γ_{eq} , which has by far the largest size [177, 170]. This fact is also known as **dominance of thermal equilibrium** and can be expressed as

$$\frac{\mu_E(\Gamma_{\text{eq}})}{\mu_E(\Gamma_E)} \geq 1 - \varepsilon \quad (2.64)$$

with $0 < \varepsilon \ll 1$.

For classical systems the Boltzmann entropy is defined as follows, let $X \in \Gamma_\nu$, then

$$S_B(X) = k_B \log \mu_E(\Gamma_\nu(X)), \quad (2.65)$$

where k_B is Boltzmann's constant. As X is the *actual* phase point of the system, micro states are directly connected to macroscopic entropy states. Further (2.65) is defined out of equilibrium, since clearly X_t can vary through different regions in phase space leading to different values of (2.65) also possibly leading to its increase. It further is extensive, such as thermodynamic entropy is and also its value in thermal equilibrium is in line with thermodynamic entropy. As by dominance of thermal equilibrium it follows that

$$S_B(X_{\text{eq}}) \approx k_B \log \mu_E(\Gamma_E). \quad (2.66)$$

With this definition of entropy one is able to explain the second law of thermodynamics [136]:

Second Law BCSM: Given $\nu \neq \text{eq}$, for most phase points $X(0) \in \Gamma_\nu$, $X(t)$ moves to bigger and bigger macro sets as t increases until it reaches Γ_{eq} , except possibly for entropy valleys that are infrequent, shallow, and short-lived; once $X(t)$ reaches Γ_{eq} , it stays in there for an extraordinarily long time, except possibly for infrequent, shallow, and short-lived entropy valleys.

Now the exceptions are fluctuations, which will not destroy the essence of the second law. There is a nice argument that makes this statement plausible, for two distinct points in time, e.g. $t_0 = 0$ and $t > 0$. Let Γ_{ν_0} be the macro region of the initial state. Via the Hamiltonian flow it will be transported to $A_t = \Phi_t(\Gamma_{\nu_0})$. Due to Liouville's theorem the volume is preserved, i.e., $\mu_E(A_t) = \mu_E(\Gamma_{\nu_0})$. The vast number of particles lead to a huge difference in phase space volumes [170] and thus the region Γ_ν is much larger than the union of all subspaces $\Gamma_{\nu'}$ which have lower entropy. More precisely:

$$\mu_E(A_t \cap \Gamma_{\text{mc}}^{\leq \nu}) \ll \mu_E(A_t), \quad (2.67)$$

where

$$\Gamma_{\text{mc}}^{<\nu} = \bigcup_{\nu': S_{\text{B}}(\nu') < S_{\text{B}}(\nu)} \Gamma_{\nu'} \cap \Gamma_{\text{mc}}. \quad (2.68)$$

Finally this means that *most* initial states $X(0) \in \Gamma_{\nu_0}$ evolve such that $S_{\text{B}}(X(0)) \leq S_{\text{B}}(X(t))$. We will see a similar argument in the quantum case at the beginning of Part II. Note that we took exactly two times, but in general we want to consider the whole history of the entropy curve.

3. Boltzmannian Framework

Boltzmann's treatment of statistical mechanics can be seen as an instance of a more general framework for understanding macro-on-micro supervenience [169, Chap. 1.4]. The aim is to explain phenomena, more precisely (macroscopic) empirical regularities, from an underlying microscopic theory by appealing to typicality. We saw in Chapter 2 how Boltzmann's statistical reasoning can explain the emergence of macroscopic regularities based on an individualist description of closed quantum systems. That is for quantum systems thermal properties can be understood in terms of wave functions and for classical systems in terms of phase points. In particular the knowledge or ignorance of an observer does not play any role here.

What we did not discuss so far is the role of the measurement problem in the BQF. Since wave functions can in general have contributions from different subspaces this leads to macroscopic superpositions. It is well known that quantum theories without observers solve the measurement problem [193, 118, 287]. Here we focus on Bohmian mechanics (BM), a non-relativistic quantum theory about point particles guided by the wave function. This theory explains the axioms of standard quantum mechanics using a Boltzmannian typicality analysis, which we explain below. This is based on the fact that BM is about point particles.

The statistical analysis of Bohmian mechanics along Boltzmann's classical ideas has been worked out by Dürr et al. [82]. There they claim the following:

“Note that it would make little sense to ask for a derivation of quantum statistical mechanics from the first principles provided by orthodox quantum theory. The very meaning of orthodox quantum theory is so entwined with processes, such as measurements, in which thermodynamic considerations play a crucial role that it is difficult to imagine where such a derivation might begin, or, for that matter, what such a derivation could possibly mean!”[82, p.891]

That might only be partly true as we show in this Chapter and also throughout the whole thesis. Ensemble typicality (see Section 1.3), the BQF (see Chapter 2) or the GAP measures are examples where the orthodox quantum formalism is enough.

Further our goal in this Chapter is to highlight the key elements of Boltzmann's statistical reasoning. They mainly rely on positing a primitive ontology (PO), a law governing the evolution of the PO and a typicality measure connected to the law allowing for an explanation of empirical regularities. Interestingly it turns out that a PO is not necessarily needed to make reasonable statements about objective

facts in nature. A typicality analysis for quantum systems (in the standard quantum mechanical formulation) with a large number of degrees of freedom is already (almost) enough (see Chapter 2 and Part III).

Both the PO versions and the “more standard” QSM share a realist attitude. That is they do not rely on an observer or the ignorance of an observer to make statements about the behavior of systems with large degrees of freedom. They describe the actual behavior of systems and are thus closely related to the realistic attitude of BM.

The closest connection of BM and orthodox quantum mechanics (OQM) might be the thermal distribution of the wave function of a subsystem. This wave function is motivated by a key quantity of BM the conditional wave function.

We start with explaining the concept of typicality in Section 3.1. In Section 3.2 we discuss Boltzmann’s reasoning on an exemplaric case: classical mechanics. After that, in Section 3.3 we go on to the quantum realm with a particular focus on the measurement problem and Bohmian mechanics. In a last step in Section 3.4 we try to build on the ideas of the last Sections, by discussing a more generic reasoning in physics: Boltzmann’s.

3.1. Typicality

The appeal to typicality stems from the aim to explain empirical regularities. These can be experiences from everyday life (not necessarily related to physics), such as realizing that almost any bobcat has a short tail [306], the equal appearance of heads and tails in a long sequence of coin flips or physical observations such as the fact that most systems evolve towards thermal equilibrium. There can of course always be exceptions, but the point is that these are extremely rare. The aim of this section is to discuss some of its key elements from a more conceptual perspective. Typicality shows a deep connection between physics, mathematics and philosophy. It is about physical phenomena that typicality reasoning refers to, it does need the mathematics of measure theory and it does need philosophical considerations as its about scientific explanations, while also digging into the question what probability actually means. So it captures a whole lot. At the same time it’s hard to entangle the different aspects of typicality. Here our aim is not to show its elements systematically, but in such a form that its essence shows of properly. In this Section we mostly follow [169].

Let us start with a definition of typicality [169, p.3]:

Definition 3.1. Let Ω be a set and Π a set of properties that the elements of Ω could possess. The set Ω is called the domain or reference set of the typicality statements. A property $P \in \Pi$ is *typical* within Ω if nearly all members of Ω instantiate P . The property is *atypical* within Ω if $\neg P$ is typical.

Here’s an example: let $\Omega = \Gamma_{\text{mc}}$ be the energy shell in phase space and P the property of being in thermal equilibrium. Then nearly all elements of Γ_{mc} have the

property P . Here's another example: let Ω be the set of lottery tickets and P the property to be a losing ticket. Then nearly all elements of Ω have the property P . For different examples, for instance from mathematics see [169, Sec.14.3].

But what does “nearly all” mean? First one can also say it differently, for instance “most” or even “with very high probability” or even call a typical phenomenon “universal”. In order to quantify the meaning of “most” in the typicality statements we need a measure. In the discontinuous case, we just count. However, for the continuous setup we need more and this is the one needed in physics. One can define typicality via a measure μ (which we define in a minute) like this [169, p.4]:

$$\text{Typ}(P) : \Longleftrightarrow \mu(\{\omega \in \Omega : P(\omega)\}) \approx \mu(\Omega). \quad (3.1)$$

Using probability measures, one understands typicality like this [9, p.82]. Let $\mathbb{P}$ be a probability measure on Ω . A claim $c(\omega)$ with $\omega \in \Omega$ is typical within Ω , if

$$\mathbb{P}\{\omega \in \Omega \mid c(\omega)\} \geq 1 - \varepsilon, \quad (3.2)$$

with $0 < \varepsilon \ll 1$. We will explain the just used notions below. Further we elaborate possibilities how such statements can be made. We will end with key results of probability theory which in the same vein are key to typicality statements.

The measure to choose depends on the physics one is considering. In general it is not too decisive which measure to take, as a typical property does not rely on it too much. As Tim Maudlin puts it [169]: “The sahara is nearly all sand.” Relative to which measure, you might ask. Area measure or volume? The point is: to both of them. The sahara is consisting of sand almost everywhere. It will be the physical law determining the measure as we explain below.

Historically typicality found its role early in the development of probability theory. Jakob Bernoulli, who stated the first version of the law of large numbers in his work *Ars Conjectandi* from 1713 [19], writes:

“Because it is only rarely possible to obtain full certainty, necessity and custom demand that what is merely morally certain be taken as certain”[120, p.3].

Another important step made in probability theory is to connect the theory with everyday life. What does that mean? Is probability about uncertainty? Whether heads or tails will appear next in a coin toss is equally probable²⁶. But what are the consequences of that. It's what Bernoulli calls “morally certain”, it refers to what should happen. Just as morality guides you toward actions you ought to take,

²⁶If you think more about it, there is actually nothing random in flipping a coin, as the laws of physics can in principle tell you what happens. One has to do a tedious calculation, but still it's possible.

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probability theory governs random “actions,” that is, random outcomes (for more details see [147, 169]).

Here’s a principle crucial for the relation of probabilities and the actual world

“A physically impossible event is one whose probability is infinitely small. This remark alone gives substance - an objective and phenomenological value - to the mathematical theory of probability.”[120, p.3]

This has become known as **Cournot’s principle** and had influence on the founding fathers of probability theory (see [120, p.3] and [169, Ch.3]). In his Grundbegriffe [162] Kolmogorov writes: “Only Cournot’s principle connects the mathematical formalism with the real world.”[120, p.3].

Typicality has not only been around in the early days of probability theory, but also in physics after the 1950s [121]. While the term “typicality” itself has not been used by the people quoted above, it has so in the context of statistical mechanics (classical (in particular by Boltzmann) and quantum) and quantum mechanics. For more details on the history see [120, 147].

Typicality and Probability

Typicality makes use of probability measures and central results of probability theory, such as the law of large numbers. However one has to keep in mind that these two notions are distinct (for details see [305, 306]). This section is a little bit more technical than the others in this chapter; here we mostly follow [169, Ch.2] and [284, Ch.3].

We start with some elementary notions from probability theory. Let Ω be a set with corresponding σ -Algebra $\mathcal{F}$ and let μ be a measure on $(\Omega, \mathcal{F})$, then $(\Omega, \mathcal{F}, \mu)$ is called a measure space. A measure $\mathbb{P}$ with $\mathbb{P}(\Omega) = 1$ is a probability measure on $\mathcal{F}$, such that the triple $(\Omega, \mathcal{F}, \mathbb{P})$ is a probability space; further for $A \in \mathcal{F}$, the number $\mathbb{P}(A) \in [0, 1]$ is called the probability of A . Here Ω is the set of elementary events $\omega \in \Omega$, these are the ones that can actually instantiate themselves.

A random variable X is a map $X : \Omega \rightarrow \mathbb{R}$. Note that there is nothing “intrinsically” random about X as it is merely a coarse-graining procedure collecting elementary events, in the sense that some $\omega \in \Omega$ get mapped to the same outcome; later on we will see that macro variables do exactly that without “being” random.

Remark 3.1.1. A natural way to understand the coarse-graining procedure and its relation to the law of large numbers is done by the so called Rademacher functions [84, 83, 169]. $\diamond$

A measure ν on $(\Omega, \mathcal{F})$ has a density function $\rho : \Omega \rightarrow [0, \infty]$ relative to the measure

κ on $(\Omega, \mathcal{F})$ if and only if ρ is measurable and

$$\nu(A) = \int_A \kappa(d\omega) \rho(\omega). \quad (3.3)$$

In the case of probability measures, we write

$$\mu(A) = \int_A \mathbb{P}(d\omega) \rho(\omega). \quad (3.4)$$

The distribution of a random variable is given by the measure $\mu(A) = \mathbb{P}(X \in A)$ and we write

$$X \sim \mu. \quad (3.5)$$

Here's an example relevant for our considerations:

Remark 3.1.2. For a classical system, thermal equilibrium in the ensemblistic view is described by the respective thermodynamic ensembles. Let us consider the canonical ensemble. As $\rho_{\text{can}}(x) = e^{-\beta H(x)}$ is the probability density of the canonical measure

$$\mu_{\text{can}} = \frac{1}{Z_{\text{can}}} \int_B dx e^{-\beta H(x)} \quad (3.6)$$

with $B \subseteq \Gamma$ and the Lebesgue measure dx . Here Z_{can} is a normalization constant and $H(x)$ the Hamilton function. Let $\mu(A)$ be the canonical measure (3.6), which is the thermal equilibrium distribution and thus a phase point on the energy surface has distribution (3.6): $X \sim \mu_{\text{can}}$; as mentioned often enough in this thesis this is how an ensemblist understands thermal equilibrium. But we will also see how we can make sense of it from an individualist perspective; especially in quantum mechanics (see Part III). $\diamond$

The expectation value of a random variable X is defined as

$$\mathbb{E}X = \int_{\Omega} X(\omega) \mathbb{P}(d\omega) \quad (3.7)$$

and the variance as

$$\text{Var}X = \mathbb{E}[(X - \mathbb{E}X)^2] = \mathbb{E}(X^2) - (\mathbb{E}X)^2. \quad (3.8)$$

The standard deviation σ_X is the square root of the variance.

There are two important inequalities, which allow to talk about the typical behavior: Markov's inequality and Chebyshev's inequality. For $\varepsilon > 0$ the former reads

$$\mathbb{P}(|X| \geq \varepsilon) \leq \frac{\mathbb{E}X}{\varepsilon}, \quad (3.9)$$

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while the latter follows from the former and is given by

$$\mathbb{P}(|X - \mathbb{E}X| \geq \varepsilon) \leq \frac{\text{Var}X}{\varepsilon^2}. \quad (3.10)$$

Hence if the variance is small, the random variable X is concentrated around a deterministic value $\mathbb{E}X$, which is then the typical value.

A key result in probability theory is the law of large numbers (LLN), which is also a key typicality statement [306, 80, 169]. There are different versions of the LLN differing in the used notion of convergence (see, e.g., [21]). We will simply refer to the LLN as this distinction is not important for us here.

What is the point we want to make here? The point is that its certainly not an overstatement that the LLN is basic to all of the Boltzmannian reasoning. The way we state it here brings several things together: it shows what role coarse graining plays, it shows that its about the empirical distribution (the actual distribution), i.e., a fact what is happening in reality, that there is an abstract theoretical distribution, which is obtained from a fitting limiting procedure and also that this convergence is given with respect to another probability measure (as we will later see a typicality measure). The role of these different measures will be made more precise below. Notice that all of the important insights are already there in an “elementary” statement of probability theory. Further we want to discuss the Maxwellian velocity distribution as an example, which is more or less a direct application of the LLN.

Let $X_1, \dots, X_N$ be independent and identically distributed (i.i.d.) random variables and denote the empirical mean as

$$m_{\text{emp}} = \frac{1}{N} \sum_{i=1}^N X_i. \quad (3.11)$$

The LLN is the following statement: let $\varepsilon > 0$, then

$$\mathbb{P}(|m_{\text{emp}} - \mathbb{E}(m_{\text{emp}})| > \varepsilon) \leq \frac{C}{N\varepsilon^2} \quad (3.12)$$

with constant $C > 0$. Thus for large enough N , such that $N \gg C/\varepsilon^2$ and suitable ε the random quantity (3.11) is close to its average value, i.e., a deterministic value. Say for example choose $\varepsilon(N) = N^{-\alpha}$ with $\alpha > 0$, then for $\alpha \in (0, 1/2)$ the right hand side in (3.12) is small and also the expression in the brackets gets small. In this way the LLN connects probabilities to the world.

Also important to mention in this context is that the standard deviation of $\sum_i X_i$

is of the order $\sqrt{N}$ and thus for the typical relative deviations one has

$$\frac{\sum_i X_i - \sum_i \mathbb{E}X_i}{\sum_i \mathbb{E}X_i} \approx \frac{1}{\sqrt{N}}. \quad (3.13)$$

Statistical mechanics make use of this in the following. First of all treating macro variables as random variables shows that the latter can be understood in terms of a coarse-graining procedure (and thus not an intrinsic randomness as the name suggests). Second assuming that these macro variables are independent (of course an idealization, as particles interact and thus loose their independency) and using the large number of degrees of freedom one can compute expectation values and declare them as the typical values.

The most famous probability distribution is the Gaussian distribution in $\mathbb{R}^d$ also known as the normal distribution denoted as $\mathcal{N}^d(\boldsymbol{\mu}, C)$, with expectation $\boldsymbol{\mu}$ and covariance matrix C . Its probability density function is given by

$$\rho(\mathbf{x}) = \frac{1}{Z} \exp \left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T C^{-1}(\mathbf{x} - \boldsymbol{\mu}) \right), \quad (3.14)$$

where Z is a normalization constant and $\mathbf{x} \in \mathbb{R}^d$.

Let us also state the **central limit theorem (CLT)** [169, p.30]. Consider for simplicity the case $d = 1$. Let $X_1, \dots, X_N$ be i.i.d. random variables with expectation μ and variance σ . Then the distribution of the random quantity

$$Y(X_i) := \sqrt{\frac{N}{\sigma}} \left(\frac{1}{N} \sum_{i=1}^N X_i - \mu \right) \quad (3.15)$$

is for large enough N given by a normal distribution $\mathcal{N}(0, 1)$.

There are also other ways to quantify the closeness of random variables to deterministic approximations, for instance through the concentration of measure phenomenon (see, e.g., [178, 48, 268, 114]). For example the instance that high dimensional spheres contain most of their volume underneath their surface (“in high dimensions oranges are mostly peel.”). Another example is the fact that two normalized random Gaussian vectors are typically orthogonal: let $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ with $\|\mathbf{x}\| = \|\mathbf{y}\| = 1$ be two independent Gaussian distributed vectors. Then for large d , typically $\mathbf{x} \cdot \mathbf{y} \approx 0$. Another example is Levy’s lemma used in Section 11.1. These results make use of the high-dimensional spaces involved and are therefore useful in statistical mechanics as the dimension is directly connected to the number of degrees of freedom. For instance in quantum mechanics where the systems state space is given by a Hilbert space $\mathcal{H}$, which usually has dimension $\dim \mathcal{H} \propto e^N$, with N the number of degrees of freedom.

Typicality Analysis

Let us elaborate a bit more on typicality reasoning. It enters physics in a particular way. Due to the large number of particles in a system, statistical physics makes use of probability reasoning (see, e.g., [254, 9]). A point that lead Smoluchowski to the following two famous questions [293](see also [84, p.50]):

- (1) How can random causes have lawlike effects?
- (2) How can lawlike causes have random effects? How does randomness emerge from determinism?

Both questions are answered by typicality [84, p.50]. The first question is answered by the law of large numbers, which is a typicality statement [307, 84, 165]. The second question is answered by Boltzmann's typicality account [170]. We come to this now. Boltzmann's reasoning serves as a more general account to explain physical phenomena. It also points out why the individualistic viewpoint is the correct one. The appearance of "randomness" is just the typical behavior. That's the end of the story. Let us explain.

Boltzmann explained why system are in thermal equilibrium by stating that most micro states are such that they represent thermal equilibrium. Regarding question (2) of Smoluchowski this means that it's the **typical behavior** that emerges macroscopically. It's how most systems behave.

If one has shown that a certain property P is typical, what are the consequences of that? Typicality statements explain what happens in most cases and are thus not deduced as a direct consequence of some law, they are not deductive-nomological explanations. Once a property has been established as typical that's the end of the story. Or stated differently: once a behavior has turned out to be typical, there is nothing left to explain. This has its foundation in the following principle [169, p.6]

Rationality Principle of Typicality (RPT): Suppose we accept a theory T and find out that our world has some salient property P .

- (1) If P is typical according to T , there is nothing left to explain. It is irrational to wonder further why our world is typical with respect to instantiating P .
- (2) If P is atypical according to T , we should look for additional explanation or, in the last resort, revise or reject the theory.

That is we have good reasons to assume that P does take place. For instance it is reasonable that isolated systems thermalize, that sequences of heads and tails roughly show a fraction of $1/2$ heads and $1/2$ tails or that entropy increases. Most importantly that these just mentioned cases *do take place in our world* and do not depend on our

ignorance or anything subjective. An atypical event has to be explained only in the case if there would have been the possibility for a typical outcome. Otherwise it is called a brute fact [169, Ch.1]. The latter does not require any further explanation, such as for example the shape of your favourite holiday island. It is just what it is, it could be different, but you would not wonder (or even realize).

It follows from the RPT that a property P is typical with respect to T , that we should expect P [169, p.7]. The role of the theory T is to lay the ground for the set of possibilities Ω . The laws suggest the typicality measure, but the typicality measure is not the crucial point (as typical behavior does not depend on the measure, think back to the sahara sand example). What is important is that dynamical evolutions in accordance with the laws are typical. In that sense the typical behavior is law like (we will get to it in a minute why they still differ).

Now the laws themselves are contingent as they could have been different and one would not realize. As soon as regular behavior is explained based on these laws, there is basically nothing more to explain [169, p.8]. Even if a creature like Laplace's demon or an angel [174] that knows everything would agree on typicality. Because it does not rely on the knowledge about a system. It does not rely on whether one knows what all the particles do, because what they do is typical anyway and therefore precise knowledge is not needed. There are initial conditions that lead to a decrease of entropy, but these are atypical. And for them being atypical it does not matter whether we know that they are atypical.

With respect to thermal behavior, one might wonder why a typicality result should be sufficient. At first glance, this seems to be a rather unsatisfactory answer—similar to the response of a parent who cannot provide a real explanation when a child asks why they have to visit their grandmother, and the father simply replies: “Because that’s what we typically do.” While this example refers to traditions—which may themselves exhibit a certain law-like structure—they remain fundamentally distinct from physical laws. Physical laws determine the range of possible histories of the universe. Explanations end with the laws. If a behavior is typical with respect to these laws, then that’s the end of the story. Still typicality is not similar to necessity, that is there are initial conditions for which a gas will do god knows what, for instance “initial conditions for which the gas will transform into a banana” [169, p.152]. But these are just extremely unlikely to happen. That is the phenomena we observe are the ones that are typical.

Let us just briefly mention the distinction between typicality and probability relevant to our discussion. The upshot is that typicality is the more fundamental notion [169, p.11]; for further details see [169, 305, 306, 307]. Here two things are important.

First referring to probability theory and its tools does not mean that there is any intrinsic randomness (the mathematical formalism is agnostic about that). The microscopic histories of systems with large degrees of freedom are determined by laws.

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Although not being feasible one can make sense of their behavior by a typicality analysis. That is in essence applying the law of large numbers to it. In particular typicality allows to make statements about the actual behavior of systems. That is, it does not rely on the role of an observer or the knowledge we have about systems. Neither for classical mechanics nor for quantum mechanics.

Second typicality means to either “go big or go home”. That is there are just two values to make sense of, either 0 or 1. That is either its typical or atypical. And because of a simple property of probability measures it does not matter whether you call “1” typical and “0” atypical or vice versa. Saying that a property is typical with typicality outcome $1/2$ is meaningless (see, e.g., [119, 169]).

One might wonder what the status of a law is, if it is only valid for most cases. Let us dwell on the second law of thermodynamics here and refer to [169, Sec.8.2] for a detailed discussion. Shouldn’t a law express a necessity? Further due to Poincaré recurrence the second law does not hold all the time. If that is the case, what is its status? Still, the second law is more than a fact, as lets say the shape of germany. Could the shape of germany be different? Of course. Would it make any difference? No (politics aside). There is something about the second law that makes us feel that it’s not an accident. Fitting between mere contingency and necessity is typicality. Now the second law holds for almost all possible worlds where the microscopic histories are determined by dynamical laws. Still not in all of them, but typicality is just an “ ε ” away.

The appeal to typicality has been criticized in the literature (see [170, 169]). A common objection refers to not being rigorous enough as there are always exceptions. One could say that it is better than nothing, and since we are not explaining the emergence of the second law by invoking wizards, witches, or other supernatural agents, we are doing reasonably well. And further this is also not wanted out of counterfactual robustness [169]. Some critics mix typicality and probability [135]. One common objection is that “most” does not mean “any” and “most” is not enough. That is there is a mix up between a logical deduction (“any”) and a physical explanation (“most”). The typicality approach has been criticized from as early on as the QET of von Neumann. It has been coined to be unphysical [24, 100]. Another misnomer is that typicality is not related to the dynamics. Let us just say that all these critique points are misguided and based on a wrong understanding of typicality, for details see [170, 165].

Remark 3.1.3 (Beyond physics). Interestingly typicality reasoning also applies in sociology [298]. That might not be surprising as societies can also be modelled or understood as complex systems. $\diamond$

3.2. Boltzmannian Reasoning in Classical Mechanics

Let us briefly discuss Boltzmann's account for classical statistical mechanics. This has largely been done in Section 2.7. Here we focus on Boltzmann's reasoning for subsystems and explain why Maxwell's velocity distribution is a typicality result. Another example in this spirit is the quantum equilibrium hypothesis [82, 84], which we explain in the next Section.

One reason we stated the LLN above is that it can be related with a famous distribution in statistical physics, namely the Maxwell-Boltzmann velocity distribution; here we follow [169, Ch.7] and [284, Ch.4].

Usually in physics we are not concerned about the evolution of the whole universe, but about subsystems. That might sound a bit strange, but in order to derive statements about subsystems one has to know what the underlying theory of the whole universe is. So suppose your theory is about classical point particles then one can consider Hamiltonian mechanics to be the fundamental theory (of course this is not the "right" theory of the universe, but that is not the point here). Then the dynamics is given by Hamilton's equations as discussed in Section 2.7. Consider a small region of such a universe, say a box $\Lambda \subset \mathbb{R}^3$ containing N non-interacting point particles (all with mass m), that is the Hamilton function reads

$$H = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m}. \quad (3.16)$$

As energy is conserved the relevant subset of phase space is

$$\Gamma_E = \Lambda^N \times \mathbb{S}_{\sqrt{2mE}}^{3N-1} \quad (3.17)$$

where $\mathbb{S}_R^d$ denotes the sphere in $\mathbb{R}^d$ with radius R . Further μ_E denotes the Liouville measure²⁷. The average energy per molecule is denoted as $\bar{E}$, such that $E = N\bar{E}$ and fixed to be $\bar{E} = \frac{3}{2}k_B T$. Now we ask: what is the fraction of particles having velocity, say in the x -direction, roughly close to $v_0 \in \mathbb{R}$? Denote $v_{i,x} = v_i$ and consider the macro variable

$$G(X) = \frac{1}{N} \sum_{i=1}^N \mathbb{1}_{\{v_i \in [v_0 - \delta, v_0 + \delta]\}}(X) \quad (3.18)$$

with $\delta > 0$ and $\mathbb{1}_A(x)$ the characteristic function. One can show that for any $\varepsilon > 0$

$$\mu_E \left(\left\{ X \in \Gamma_E : \left| \frac{1}{N} \sum_{i=1}^N \mathbb{1}_{\{v_i \in [a,b]\}}(X) - \int_a^b dv \rho_{\text{Max}}(v) \right| > \varepsilon \right\} \right) \approx 0 \quad (3.19)$$

²⁷Here we do not care about the difference between the measure on the energy surface Γ_E and the measure on the energy shell $\Gamma_{E,\Delta E} = \{X \in \Gamma : E - \Delta E \leq H(X) \leq E\}$.

3. Boltzmannian Framework

for $N \gg 1$. Where

$$\rho_{\text{Max}}(v) = \left(\frac{2\pi k_{\text{B}} T}{m} \right)^{-1/2} \exp \left(\frac{-mv^2}{2k_{\text{B}} T} \right) \quad (3.20)$$

is the Maxwell velocity distribution. What is important here to mention are the different roles of the probabilistic notions made in this paragraph. First of all the fact that one derives a probability distribution for the velocity of the particles does not mean that there is something random going on. It means that most microscopic configurations are such that their velocity distribution is close to the Maxwellian. This was already highlighted by Boltzmann (translation [284, p.33]):

“The case that all molecules have exactly the same velocity in the same direction is no more improbable than the case that every molecule have exactly the velocity and direction that it actually has in the gas in a certain instant. However, if we compare the former case to the case that the Maxwellian distribution of velocities applies, then we find again that the latter case comprises many more equally possible cases.”

Boltzmann does not say typical but he refers to “many more equally possible cases”.

What this derivation also shows is the connection between the empirical distribution given through $G(X)$, the theoretical distribution ρ_{Max} and the typicality measure μ_E . That is the typicality measure connects the *actual* velocity distribution of the particles with a theoretical distribution (in the large N limit). And therefore (3.20) is typical; for more details see [169, 120]. The Maxwellian velocity distribution (3.20) can be deduced using the maximum entropy principle (MEP) (see Section 11.2). For the MEP however the knowledge or ignorance about a system plays a crucial role. As a consequence of the result above the role of knowledge we have about the system does not play any role. That is we have explained a fact of nature using typicality reasoning.

What might also be worth to mention here is the coarse-graining procedure introduced in $G(X)$. We did not ask, what the distribution of the *precise* velocity of the particles is. That would have lead us to conclude that its zero. This is of no particular physical meaning. It is just an instance of the mathematical fact that points have measure zero. Thus coarse-graining is essential.

At this point we can also mention how to make sense of ensembles in the individualistic view for classical systems; we follow [165, p.159].

Suppose in a universe U there are n independent copies of subsystems S all with the same Hamilton function H ; the rest of U (environment) of the universe is denoted as $E = U \setminus S$. Now split the phase point into the ones belonging to S and to E , such

that $X = (X^S, X^E)$ and further $X_S = (X_1^S, \dots, X_n^S)$. Define a macro variable M on S as follows

$$M_{\text{emp}}^n(X) = \frac{1}{n} \sum_{i=1}^n M(X_i^S), \quad (3.21)$$

for example the macro variable defining the actual distribution of phase points in $A \subseteq \Gamma^S$, i.e., $M(x) = \mathbb{1}_A(x)$ and therefore (3.21) would express the relative frequency of ensemble systems with phase points in A . A typicality result, in which one would be interested would be of the form (e.g. the Maxwellian)

$$\text{Typ} \left(X^S : M_{\text{emp}}^n \approx \int dX^S M(X^S) \rho(X^S) \right). \quad (3.22)$$

This is derived from a LLN argument, namely

$$\mu_E \left(X \in \Gamma_E : \left| M_{\text{emp}}^n - \int dX^S M(X^S) \rho(X^S) \right| > \varepsilon \right) \leq \delta(\varepsilon, n, M) \quad (3.23)$$

in such a limit that $\delta(\varepsilon, n, M)$ will get sufficiently small for large enough n . Here μ_E denotes the micro-canonical measure (of the “universe” U). The conceptual meaning of these results is that ensembles are best understood in terms of typicality. They have nothing to do with randomness. Classical thermodynamic ensembles designate the set in phase space as the set of points that show up on a macroscopic level like typical (“ ρ -most”) phase points [136, Sec.7.3].

Results of this kind can be derived for quantum systems (see Part III below in this Chapter).

3.3. Boltzmannian Reasoning in Quantum Mechanics

3.3.1. Macroscopic Entropy Superpositions

We have seen in Chapter 2 that the BQF provides a coherent setting to describe thermal equilibrium and thermalization. However, a state $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ can be in a superposition of contributions in different subspaces, namely

$$\psi = \sum_{\nu \in \mathcal{N}} \hat{P}_\nu \psi. \quad (3.24)$$

Then define for example the entropy operator via

$$\hat{S}_{\text{QB}} = \sum_{\nu \in \mathcal{N}} S_{\text{QB}}(\nu) \hat{P}_\nu, \quad (3.25)$$

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where the quantum Boltzmann entropy $S_{\text{QB}}(\nu)$ (see (4.13)) appears as an eigenvalue (up to now we have not discussed entropy, but we will need it below and therefore we use it as a macro variable here.). Now ψ can also be in a superposition of different entropy values. Hence which entropy values does the system actually have? In standard quantum mechanics this problem is solved by the projection or collapse postulate (see e.g. [245, 138, 237] here we follow the presentation in [287]²⁸). If a measurement of “the entropy $\hat{S}$ ” (actually one “measure” the operator, whatever that means (for a discussion see, e.g., [287, 84])) for a system in state ψ (before the measurement) is made and the outcome $S_{\text{QB}}(\nu)$ is obtained, then after the measurement the state of the system with probability $||\hat{P}_\nu\psi||^2$ given by

$$\psi' = \frac{\hat{P}_\nu\psi}{||\hat{P}_\nu\psi||}, \quad (3.26)$$

where $\hat{P}_\nu$ is the projector onto the eigenspace of $S_{\text{QB}}(\nu)$. The collapse of the wave function is described by Dirac as follows: “[a] measurement always causes the system to jump into an eigenstate of the dynamical variable that is being measured.”[78, p.36]. It does not require any further elaboration in the orthodox view and is taken to be “one of the fundamental postulates of quantum mechanics, so it cannot be proven”[237, p.24]. That might be the case in the standard textbook version of the theory, but it certainly is not the case for “quantum theories without observers” [118].

Here foundational issues of statistical mechanics and quantum mechanics come together in form of the measurement problem. We do expect an actual macroscopic entropy value of the system and not several possible entropy values waiting to be observed.

Let us elaborate a bit more on how the measurement problem in a statistical physics setting looks like (see, e.g., [15, 3, 84, 83, 33, 287, 203, 169] for general treatments of the measurement problem). Suppose you are given a macroscopic system and you should find out whether its in thermal equilibrium or not, that is whether the entropy value is $S_{\text{QB}}(\text{eq})$ or $S_{\text{QB}}(\text{neq})$. That means the respective energy shell is decomposed into two subspaces $\mathcal{H}_{\text{neq}}$, corresponding to non-equilibrium and $\mathcal{H}_{\text{eq}}$, corresponding to equilibrium²⁹. You have a measurement apparatus which consists of a display and a pointer, which can point to a ready state, to “eq” or to “neq” (think of the pointer as the measurement result). That is the total system under consideration is the apparatus and the system which state is being measured.

The system is described by two states ψ_{eq} and ψ_{neq} for which the apparatus can

²⁸Consider for simplicity observables with discrete eigenvalues and an idealized measurement having “no duration”.

²⁹There might be subtleties assigning such a state in a Bohmian version of the BQF, but for the sake of the argument here, we omit these.

show whether the system is in state ψ_{eq} or ψ_{neq} (after an interaction with the apparatus). Let the state of the apparatus be given by either Φ_{eq} or Φ_{neq} (pointer positions “eq” and “neq”), where Φ_{eq} and Φ_{neq} have disjoint support³⁰ in configuration space $\mathbb{R}^{3N}$ (see definition in 3.3.2), i.e., $\text{supp } \Phi_{\text{eq}} \cap \text{supp } \Phi_{\text{neq}} \approx 0$. Further suppose that initially the apparatus is in a ready state Φ_0 (in terms of pointers, its pointing at “zero”, is in the middle between “eq” and “neq”). Now the Schrödinger evolution is such that

$$\psi_i \Phi_0 \rightarrow \psi_i \Phi_i. \quad (3.27)$$

The systems state is in a superposition

$$\psi = c_{\text{eq}} \psi_{\text{eq}} + c_{\text{neq}} \psi_{\text{neq}} \quad (3.28)$$

with $c_{\text{eq}}, c_{\text{neq}} \in \mathbb{C}$ and $|c_{\text{eq}}|^2 + |c_{\text{neq}}|^2 = 1$. This means that, again by the Schrödinger evolution,

$$\psi \Phi_0 \rightarrow c_{\text{eq}} \psi_{\text{eq}} \Phi_{\text{eq}} + c_{\text{neq}} \psi_{\text{neq}} \Phi_{\text{neq}}. \quad (3.29)$$

The severe implication of this is that macroscopically the apparatus is in a superposition of a pointer pointing at “eq” and a pointer pointing at “neq”. That means S_{QB} does not have an actual value, but is in a superposition of macroscopically different entropy values $S_{\text{QB}}(\text{eq})$ and $S_{\text{QB}}(\text{neq})$. In standard quantum mechanics the system would collapse into one the two possible values by measurement or observation. It is highly unclear why an “observer” or a “measurement” should play a role for what actually happens in the physical world.

That this has alarming consequences has been famously pointed out by Schrödinger and his cat in a series of articles in 1935 [240]. As the introduction of the projection postulate does not clarify what counts as a measurement. Iconically stated by Bell:

“It would seem that the theory is exclusively concerned about ‘results of measurement’, and has nothing to say about anything else. What exactly qualifies some physical systems to play the role of ‘measurer’? Was the wavefunction of the world waiting to jump [collapse] for thousands of millions of years until a single-celled living creature appeared? Or did it have to wait a little longer, for some better qualified system ... with a Ph.D.? If the theory is to apply to anything but highly idealised laboratory operations, are we not obliged to admit that more or less ‘measurement-like’ processes are going on more or less all the time, more or less everywhere? Do we not have jumping then all the time?”([17], p.216)

In the same vein one could ask with respect to our setting above: why is the notion of measurement relevant for a system having an entropy value that corresponds with its thermal equilibrium value? Maybe from an instrumentalist perspective this seems

³⁰Recall that the support of a function $f(x)$ is the set of x where $f(x)$ does not vanish.

fine. But that is certainly not what physics should be about. It should not just care about the outcomes of measurements without understanding what is “really” happening. With the quote of Bell in mind we think of heat flowing from the hotter to cooler not depending on whether such a scenario is observed or not, or measured or not. It simply does happen in nature and a physical explanation has to account for that!

And even worse, than the projection postulate is the statement by Pascual Jordan saying that “[o]bservations not only disturb the system what is to be measured, they produce it...We compel [the particle] to assume a definite position.”³¹ What is meant by production here is not entirely clear. It could mean that the quantum state is produced, in the sense of the collapse postulate. It could also be meant that a pure possibility comes “into being”. A ridiculous statement concerning physics.

Nowadays in its most precise form the measurement problem is stated as a logical inconsistency between the following three propositions (originally see [193], here we follow [287, 169]):

- (1) The physical state of the system is completely described by the wave function ψ .
- (2) The time evolution of ψ is given by the Schrödinger equation.
- (3) A measurement has a definite outcome.

That is, a coherent formulation has to reject at least one of these three points (for a detailed discussion see [83, 169, 287]).

Denying that the description in terms of ψ is complete leads to theories including further variables besides the wave function, such as Bohmian mechanics [82, 84].

Denying that ψ evolves unitarily leads to collapse theories, such as GRW theory (named after Ghirardi, Rimini and Weber [113]).

Denying that a measurement has a definite outcome leads to many world theories, originally proposed by Everett [98]. Note that there are also other approaches tackling the measurement problem, but we do not consider them here (see, e.g., [287] for a discussion).

So what does all of this have to do with entropy increase? Well as discussed in this section, one has to have a clear view regarding solutions to the measurement problem in order to formulate a second law of thermodynamics for closed quantum systems. We will do so for Bohmian mechanics below in Chapter 8. We leave it as an open question further to be investigated, whether a second law can also be stated in collapse models or many worlds theories.

³¹This is cited from [138, p.5]. However [138] cites a paper by Mermin [199], who refers to a book by Jammer [150, p.161]. In the book by Jammer one can find the original citation, but still not quite as it is cited as “op. cit.” and could not be found by the author.

We now discuss BM. We focus on the role of the particle ontology and Boltzmann's reasoning applied to such a theory.

3.3.2. Bohmian Mechanics

BM is a non-relativistic quantum theory about the motion of massive point particles in three dimensional space and can be considered as a fundamental theory of the universe [169] (in the sense that its coherent and objective, not in the sense that its the "final" theory). That is, we consider a system of N particles, where $\mathbf{Q}_i(t) \in \mathbb{R}^3$ is the position of the i -th particle with mass m_i and $Q(t) = (\mathbf{Q}_1(t), \dots, \mathbf{Q}_N(t)) \in \mathbb{R}^{3N}$ its configuration. Here $\mathbb{R}^{3N} = \mathcal{Q}$ is called configuration space. The state of a Bohmian universe is given by³²

$$(Q(t), \Psi_t) \in \mathcal{Q} \times \mathcal{H}, \quad (3.30)$$

with $\Psi_t : \mathbb{R}^{3N} \rightarrow \mathbb{C}$ the wave function of the universe evolving according to Schrödinger's equation

$$i \frac{d\Psi_t}{dt} = \hat{H}\Psi_t, \quad (3.31)$$

where we assume that the Hamiltonian $\hat{H}$ contains potentials (see (1.3)), which exclude configurations that might lead to divergences³³. The position of each particle evolves in time according to the guiding law [79, 16, 25]

$$\frac{d\mathbf{Q}_i}{dt} = \frac{1}{m_i} \text{Im} \frac{\nabla_i \Psi_t}{\Psi_t}(Q(t)), \quad (3.32)$$

where ∇_i is the gradient with respect to the three coordinates of the i -th particle. Note that one can think of $\mathcal{Q} \times \mathcal{H}$ with $\mathcal{H} = L^2(\mathbb{R}^{3N}, \mathbb{C})$ as the phase space of BM [79]. That is BM consists of two dynamical equations. BM is time reversible: if $t \mapsto (Q(t), \Psi_t)$ is a solution of the equations of motion (guiding law and Schrödinger equation), then $t \mapsto (Q(-t), \Psi_{-t}^*)$ is also a solution of the equations of motion.

The time evolution is well-defined [18, 276]. The guiding law can be stated more compact

$$\frac{dQ}{dt} = v^{\Psi_t}(Q(t)) \quad (3.33)$$

using the Bohmian velocity field v^{Ψ_t} . This is an ordinary differential equation, which means that given an initial configuration $Q(t_0)$ and wave function Ψ_{t_0} at time t_0 the evolution $t \mapsto Q(t)$ is determined for all t . That is BM is a deterministic theory. Randomness enters in BM as follows.

³²Compare with the discussion in Chapter 3. The PO is given by point particles and their position.

The guiding law $\mathcal{L}$ by the wave function Ψ_t .

³³Note that we consider spinless particles, but the formalism can be generalized for particles with spin, see, e.g., [287, 84].

3. Boltzmannian Framework

If initially, say at time $t = 0$ (the big bang), the configuration is such that $Q(0)$ is random with probability density $|\Psi_0(q)|^2$, then $Q(t)$ has probability density $|\Psi_t(q)|^2$. This property is known as equivariance (see, e.g., [287, Sec.1.6.2]). Note here that we write Q for the actual configuration and q as a configuration variable, for instance in $\Psi(q)$ or $\rho(q) = |\Psi(q)|^2$. It is a consequence of equivariance that μ^Ψ with density $|\Psi(q)|^2$ is an invariant measure. Let $\Phi_{t,0}^\Psi$ be the flow induced by the guiding equation (3.32), then for $A \subseteq \mathbb{R}^{3N}$

$$\mu^\Psi(A) = \int_A d^{3N} |\Psi_0|^2 = \int_{\Phi_{t,0}^\Psi(A)} d^{3N} |\Psi_t|^2. \quad (3.34)$$

Equivariance is analogous to the stationarity of the Liouville measure in classical mechanics. An thus (3.34) serves as a natural measure to make typicality statements.

One of the most important traits of BM and relevant to us here is that it solves the measurement problem [287, 169], which we described in Section 3.3.1. The reason is mainly due to relying on a particle ontology as particle positions selecting a possible macroscopic state, that is the particles “being somewhere” (for a discussion see [287]). Here’s what it means with respect to our situation described in Section 3.3.1: the probability given that $Q \in \text{supp}(\psi_{\text{eq}})^{34}$ is given by

$$\mathbb{P}(Q \in \text{supp}(\psi_{\text{eq}})) = \int_{\text{supp}(\Psi_{\text{eq}})} dq |\psi(q)|^2 = \int_{\mathbb{R}^{3N}} |c_{\text{eq}} \Psi_{\text{eq}}|^2 = |c_{\text{eq}}|^2. \quad (3.35)$$

Although the wave function being in a superposition, the actual particle configurations determine the outcome of the measurement as they should: it is simply a fact where the particles are. Now (3.35) shows that BM yields the same probabilities for measurement outcomes as the standard quantum formalism.

Let us comment on the importance of the particle ontology here. A physical theory should be about something. Here we think of this as some sort of “stuff” located in three dimensional space $\mathbb{R}^3$. Whether that “stuff” are quarks, superstrings or atoms is not so important, what is important is that there *is* something fundamental to the theory having an objective reality making up the macroscopic world. That part of the theory is called the **primitive ontology (PO)**. A term first introduced by Goldstein et al. [82]:

“What we regard as the obvious choice of primitive ontology—the basic kinds of entities that are to be the building blocks of everything else (except, of course, the wave function) - should by now be clear: Particles, described by their positions in space, changing with time - some of which, owing to the dynamical laws governing

³⁴Here $\text{supp}(f)$ denotes the support of a function $f(x) : \mathbb{R}^d \rightarrow \mathbb{C}$, which is the set where f does not vanish. More explicit: $\text{supp}(f) = \{x \in \mathbb{R}^d | f(x) \neq 0\}$, where $\bar{A}$ denotes the closure of a set A .

their evolution, perhaps combine to form the familiar macroscopic objects of daily experience.”[82, p.850]

It is called primitive and not only ontology, because it does not account for all there is, i.e., not everything of the ontology. It simply includes the fundamental physical objects, but it for instance does not include physical laws [5]. The PO is metaphysically fundamental as it does not rely on a more fundamental basis [172]. In general the idea is quite old: the ancient greeks, in particular Leucipp and Demokrit [181, Ch.1] called the PO *atom*; see also the nice book by Schrödinger [242] and the influence of atomism for the modern world view [264].

The PO approach clears up with the quantum paradoxes. For more details on the decisive role of a PO in a physical theory see [172].

Quantum Equilibrium Hypothesis

The Born rule is empirically well justified, although conceptually it is not. We now describe how the Born rule can be explained from BM; we closely follow [169, Ch.13] (for a detailed discussion see [83, Ch.4]).

Let us briefly look at how the Born rule applies to the measurement problem. Let $q = (x, y)$ denote the possible configuration $x \in \mathbb{R}^k$ of the measured system and $y \in \mathbb{R}^m$ of the apparatus. The pointers have disjoint support in configuration space and thus by the Born rule

$$\mathbb{P}(\text{pointer at “eq”}) = \int_{\text{supp}\Phi_1} dx^k dy^m |c_{\text{eq}}\psi_{\text{eq}}\Phi_{\text{eq}} + c_{\text{neq}}\psi_{\text{neq}}\Phi_{\text{neq}}|^2 \approx |c_{\text{eq}}|^2. \quad (3.36)$$

Now in BM this probability is related to the actual particle configurations as we saw above. In OQM these probabilities refer to the possible measurement outcomes, i.e., if a measurement were performed the outcome “pointer at “eq”” would have probability $|c_{\text{eq}}|^2$. But that has nothing to do with actuality, only with possibility. Also in other quantum theories without observers these probabilities have different meanings [169, Sec.13.2].

Now we use a Boltzmannian argument from above and apply it to Bohmian mechanics to explain the Born rule. Thereby making use of the particle ontology as in the classical case, where the particle ontology is more obvious (although not to Boltzmann’s contemporaries). Considering isolated subsystems is more subtle in quantum mechanics as there is entanglement. We will see below how to take care of that.

Consider a subsystem with $n < N$ particles such that the total configuration space reads $\mathbb{R}^{3N} = \mathbb{R}^{3n} \times \mathbb{R}^{3(N-n)}$. Denote with $q = (x, y)$ the possible configurations and $Q = (X, Y)$ the actual configuration. Thus the wave function of the universe reads $\Psi_t(q) = \Psi_t(x, y)$. What we need is a wave function for the subsystem. In BM there’s

3. Boltzmannian Framework

a natural notion for the wave function of the subsystem, called the **conditional wave function** defined as follows

$$\psi_t^Y(x) := \mathcal{N}\Psi_t(x, Y), \quad (3.37)$$

where $\mathcal{N}$ is a normalization constant. That is, the subsystem is defined by the actual configuration of the environment. Usually the subsystem decouples from the environment, which allows to come up with an **effective wave function** φ

$$\Psi(x, y) = \varphi(x)\chi(y) + \Psi^\perp(x, y), \quad (3.38)$$

where χ and $\Psi^\perp$ have macroscopically disjoint y -supports and $Y \in \text{supp}\chi$, such that $\Psi^\perp(x, Y) = 0$ and therefore $\psi(x, Y) = \varphi(x)\chi(Y)$. Now φ follows its “own” Schrödinger equation and has a respective guiding equation expressed via X and. The effective wave function is the one the Born rule in OQM refers to. One should also mention that the conditional wave function leads naturally to the collapsed wave function of a subsystem (the universal wave function does not collapse), for which in OQM an observer or a measurement has to be introduced [84, Ch.11].

The goal is to explain the Born rule using typicality reasoning. Recall that for a system (the subsystem defined above with n particles) with wave function φ the particle configuration Q to lie in $A \subset \mathbb{R}^{3n}$ is given with probability

$$\mathbb{P}^\varphi(Q \in A) = \int_A |\varphi|^2(\mathbf{q}_1, \dots, \mathbf{q}_n) d^{3n}q_1 \dots d^{3n}q_n. \quad (3.39)$$

That is we need a typicality measure in order to show that the Born rule is typical. Further it should be a measure that does take the actual configuration of the environment into account.

This leads to considering the conditional measure

$$\mu^\Psi(X \in d^{3n}x | Y) = \mathcal{N}' |\Psi(x, Y)|^2 d^{3n}x = |\psi^Y(x)|^2 d^{3n}x \quad (3.40)$$

with normalization constant $\mathcal{N}'$. Under the considerations above the conditional wave function is given by the effective wave function. Further noting that a lot of different Y configurations yield the same wave function for the subsystem one finds that (for more details see [83, p.90][169, Ch.13] or [84, Ch.11])

$$\mu^\Psi(X \in d^{3n}x | \psi^Y = \varphi) = |\varphi|^2 d^{3n}x. \quad (3.41)$$

In order to apply the law of large numbers we have to consider a collection $X_1, \dots, X_M$ of M independent subsystems (think of them as M i.i.d. random variables) with wave function φ . Denote $X_i \in \mathbb{R}^{3n}$ the actual configuration of the i -th subsystem. The conditional wave function is now a product $\psi^Y(x_1, \dots, x_M) = \varphi(x_1) \dots \varphi(x_M)$ and

thus (3.41) becomes

$$\mu^\Psi(\{Q = (X, Y) : X_1 \in d^n x_1, \dots, X_M \in d^n x_M | \psi^Y = \otimes^M \varphi\}) = \prod_{i=1}^M |\varphi(x_i)|^2 d^n x_i. \quad (3.42)$$

Let $A \subset \mathbb{R}^{3n}$ and $\mathbb{1}_{\{X_i \in A\}}$ with empirical distribution

$$\rho_{\text{emp}}^M(A) = \frac{1}{M} \sum_{i=1}^M \mathbb{1}_{\{X_i \in A\}} \quad (3.43)$$

$$\mu^{\Psi_t} \left(\left\{ Q : \left| \frac{1}{M} \sum_{i=1}^M \mathbb{1}_{\{X_i \in A\}}(Q) - \int_A |\varphi(x)|^2 \right| < \varepsilon \right\} \right) \approx 1 \quad (3.44)$$

as $M \gg 1$.

The upshot is this: typical configurations Q of the universe are such that the actual configuration of particles in a collection of subsystems with wave function φ have distribution $|\varphi|^2$.

There is an actual distribution regarding the state of a microscopic system. The typicality measure connects the empirical or actual distribution μ_{emp} (here ρ_{emp}^M) with a theoretical distribution μ_{th} (here $|\varphi|^2$); note that positing a theoretical distribution before a typicality analysis is also called a “statistical hypothesis” [84, 165]. In both of the cases above the empirical distribution is given with respect to the micro state. In particular the above statements do not depend on the knowledge of an observer [169, p.127].

Notice that the QEH is a typicality statement and has the form [169, p.272]

$$\text{Typ} \left(\rho_{\text{emp}}^M(A) \approx \int_A |\varphi(x)|^2 \right) \quad (3.45)$$

Let us briefly make some remark, comparing Boltzmann’s reasoning in classical and quantum mechanics. In classical mechanics the dynamics is governed by the Hamiltonian $H = H^S + H_{\text{int}}$, while in BM the particles are governed by the wave function $\Psi = \varphi\chi + \Psi^\perp$. In both cases approximations are such that $H \approx H^S$ (the Hamilton function of the subsystem S) and $\Psi \approx \varphi\chi$. Both of these laws, yield a typicality measure, the Liouville measure $\mu_E = \delta(E - H(X))dX$ and the equivariant measure $\mu^\Psi = |\Psi|^2 d^{3N}q$. With this one can derive typical empirical distributions, such as the velocities of point particles to be close to the Maxwell distribution (or the canonical distribution) and the Born rule. It should be noted that both of these theories rely on a PO. The PO follows a deterministic law, that allows to define a typicality measure. Then by a statistical analysis using the typicality measure one

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can deduce theoretical distributions and thus *explain* these.

Furthermore, it might be confusing as $|\Psi|^2$ and $|\varphi|^2$ look the same, that one has cheated and just concluded by using the premise. This is not true.

Although not as obvious as for the Born rule, one can make a similar remark about the canonical distribution. The canonical distribution can be derived from the micro-canonical distribution by tracing out the degrees of freedom of the bath. However that would only yield the canonical distribution on average and not make it the typical distribution (a point we come back to in Part III).

The upshot of the last two chapters is that a PO, a law governing it and a statistical analysis of such a theory explain empirical regularities. It might be interesting to know whether there are other theories to apply this to.

3.3.3. Boltzmann Bohm Framework

A proper framework of QSM taking the measurement problem into account would be to connect the BQF and BM, which one could coin Boltzmann-Bohm framework (BBF); see [82, p.891] anticipating such a direction. Let us sketch some thoughts here.

The benefits of such a theory are obvious as they align with the benefits of BM and with the benefits of the BQF. In particular the BBF would be a candidate for a coherent theory describing the thermal behavior of a many particle system, while at same time solving the measurement problem. That is, it makes sound objective predictions and explains emergent behavior based on a typicality analysis. It brings together the notion of a PO, a law governing the PO and a measure allowing to make typicality assertions. Further it explains all the ad hoc principles of quantum mechanics and quantum statistical mechanics. Also the role of operators is clearly put in BM (see, e.g., [287, 84]). Could one ask for more?

However, there are at least three problems that arise. First of all macroscopic superpositions have to be taken into account. Second, even if there are none, one has to show that this will be the case as time evolves (see [9, p.114]). And third in BM particles do have an actual configuration, but cases can be constructed where different macro states ν and ν' do not have disjoint supports in configuration space. If the particle configuration Q would choose a unique macro state, this should not be the case.

Above we defined the state of a Bohmian universe as $(Q(t), \Psi_t)$. Applying this to the BQF setup the macro state ν_t at time t of a Bohmian universe would thus be given by

$$\nu_t = \nu(Q(t), \Psi_t). \quad (3.46)$$

How do the corresponding macro spaces look like? Let $Q \in \mathcal{Q}$ with the configuration space $\mathcal{Q}$ and let $\Psi \in \mathbb{S}(\mathcal{H})$ with $\mathcal{H} = \bigoplus_{\nu} \mathcal{H}_{\nu}$. In general the universal wave func-

tion is in a superposition: $\Psi = \sum_{\nu} \hat{P}_{\nu} \Psi$. Under the reasonable assumption (counter examples can be constructed, but these are unrealistic (see [136])) expected to hold for realistic systems different $\hat{P}_{\nu} \Psi$'s do not overlap in configuration space, i.e.,

$$\text{supp}(\hat{P}_{\nu} \Psi) \cap \text{supp}(\hat{P}_{\nu'} \Psi) \approx \emptyset \quad \text{for } \nu \neq \nu' \quad (3.47)$$

and therefore a well defined particle configuration, say uniformly distributed in a container, can be given. Now Q does select a unique macro state ν and in this case $Q \in \text{supp}(\hat{P}_{\nu} \Psi)$. That allows us to define as a macro region $\mathcal{M}_{\nu}$ (“analogous” as for classical systems)

$$\mathcal{M}_{\nu} = \{(Q, \Psi) \in \mathcal{Q} \times \mathbb{S}(\mathcal{H}) : Q \in \text{supp}(\hat{P}_{\nu} \Psi)\}. \quad (3.48)$$

Note that the pair $(Q(t), \Psi_t)$ is the analog of a phase point X in classical mechanics. Note further that $\mathbb{S}(\mathcal{H})$ can now be a suitable L^2 -space, say $L^2(\mathbb{R}^{3N})$.

The aim would now be to treat these sketched ideas more properly and also discuss for instance thermalization. We will not do this here. Below we discuss how one can understand the second law of thermodynamics in a Bohmian universe (see Section 8).

3.4. Boltzmannian Reasoning in Physics

The goal of physics is to come up with a theory T that might be true³⁵, in the sense that T provides a coherent setting to explain observations in an objective manner. Bohmian mechanics (BM) might be such a theory [172, 285]. As we saw BM solves the measurement problem by appealing to point particles as the cornerstones of a non-relativistic quantum theory and further BM explains the principles of orthodox quantum mechanics (OQM) such as the Born rule and the collapse postulate based on a typicality analysis.

Interestingly several seminal results in quantum statistical mechanics make objective statements, but do not necessarily rely on a PO. These include “canonical typicality” and the so called GAP measures (see Part III). Although not having a PO, a typicality analysis allows to explain the appearance of the thermodynamic ensembles.

Both approaches, with and without PO have the same aim, that is to describe and explain what happens in reality making use of a typicality analysis.

Actuality

The central aspect of Boltzmann’s reasoning is that its realistic. That means the statements one makes are about an objective reality and about individual systems.

³⁵Such a theory T does not have to be the “final” theory.

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Above we have seen that for classical systems as well as BM positing a PO is crucial to explain foundational problems. Based on the large number of degrees of freedom a typicality analysis provide the right insides. Typicality assertions are about objective facts in nature.

We also mentioned that a PO is not needed to get satisfying results. For example in Appendix 11.2 we explain why the grand-canonical ensemble appears in nature.

OQM has a positivistic attitude as one only cares about the correct outcomes of measurements, but not the reason behind those. Opposed to that is the attitude in BM, which explains the ad hoc principles of OQM, based on a realistic attitude that there are actual particles. Interestingly the fundamental quantity of OQM, the wave function ψ is itself not measurable (see, e.g., [287]). Then one might ask what the status of ψ is in a theory based so heavily on measurements.

Interestingly similar spirits appear in QSM. An ensemblist can, based on the principle of a priori equal probabilities or the maximum entropy principle make sense of the statistics of measurement outcomes for observables in thermal equilibrium. However, neither of those principles *explains* why these outcomes and not any other outcomes appear. Opposed to that is the realistic position in the BF. One can reasonably explain the essence of thermal equilibrium by appealing to typicality.

We saw that in the BQF thermalization is understood in terms of wave functions. We will also see that entropy increase can be understood in terms of wave functions and we will further see that thermal properties of subsystems can be understood in terms of wave functions. This is motivated by the fact that we aim to treat individual systems and not ensembles (see also Chapter 1). In particular this means that there is an **actual state** a system is in. And that the physical behavior and the analysis is about the behavior of this actual state. That is for classical statistical mechanics, where the actual state of a system is perfectly described by a point X in phase space, instead of a probability density $\rho(x)$ on phase space, which is usually interpreted as the degree of belief that the actual phase point is $x = X$. Thermal equilibrium should be understood from the actual state X and not from the knowledge or ignorance we have about how close a probability distribution to our knowledge is to the respective thermodynamic ensemble [128, 136].

Similar thoughts apply for quantum systems. Here the role of X is played by a wave function ψ , which is then considered as the actual state of the system instead of a statistical mixture expressed by a density matrix³⁶. Leaving this aside for a minute also wave functions ψ can be sampled according to some probability measure μ , i.e., $\psi \sim \mu$. From an ensemblist point of view μ corresponds to the subjective ignorance. Quantum systems do have limitations to knowledge, that means even the best apparatus can not resolve these. That is different to classical mechanics, where

³⁶It should be mentioned that one has to be a bit more careful here. The analog of X in QM would be (Q, Ψ) [128, 136].

in principle, building a good enough machine would help. Still that doesn't mean that wave functions can not properly describe thermal equilibrium or thermalization. They do, as we argue below in Part III for subsystems and they do also for closed systems as we have seen above in Chapter 2. We think of μ as a typicality measure and this provides us to make statements about what happens in nature for most wave functions.

In Part III we explain why ensembles are typical and also elaborate on the typical distributions of wave functions of subsystems. The results shown there and in Appendix 11.2 are of the following form. Consider a spatial region $\Lambda \subset \mathbb{R}^3$. Let $S \subset \Lambda$ and $B = \Lambda \setminus S$ with respective Hilbert space $\mathcal{H}^S$ and $\mathcal{H}^B$, such that the total Hilbert space of Λ is $\mathcal{H} = \mathcal{H}^S \otimes \mathcal{H}^B$. Assume there is some mechanism, which distributes $\psi \in \mathbb{S}(\mathcal{H})$ according to a probability measure μ , i.e., $\psi \sim \mu$, such that we “do not know” the precise state ψ . In such a case the common approach is to assign the state of a system by a density matrix and then derive the thermodynamic ensembles using the maximum entropy principle (MEP) (see Section 11.2). There the Gibbs entropy is understood as the lack of knowledge or the ignorance an observer has about a system. Under certain data, such as the expectation values of, say energy, one can derive the canonical ensemble by maximizing the Gibbs entropy under the constraints given by the known data. That is thermal equilibrium ultimately relies on the knowledge of an observer. But what if there is no observer? What about thermal equilibrium on distant planets or place we do not look at? We argue below in Section 11.2 and in Appendix 11.2 that such a view is not satisfying.

We think of thermal equilibrium differently. We think it's the typical property of a system. It's the state that most micro states realize. That is we think of the probability measure μ as a *typicality measure*. This will serve us two purposes. We will be able to coin reduced density matrices as arising typically, as well as wave functions of subsystems having typical thermal equilibrium distributions. Let us dwell on these two points for a moment.

First, it will allow us to understand the emergence of the micro-canonical ensemble (and therefore also the canonical ensemble). It will also allow us to understand the foundations of the grand-canonical ensemble and the so called generalized Gibbs ensembles (see Appendix 11.2). That is we discuss typicality statements of the following form: let $\psi \sim u_{\mathbb{S}(\mathcal{H}^R)}$, where $\mathcal{H}^R \subset \mathcal{H}$ is a suitable Hilbert space and $u_{\mathbb{S}(\mathcal{H}^R)}$ the uniform distribution on $\mathbb{S}(\mathcal{H}^R)$. Then it is known (“canonical typicality”, see, e.g., [214, 133]) that for most $\psi \in \mathbb{S}(\mathcal{H}^R)$

$$\mathrm{tr}^B |\psi\rangle\langle\psi| \approx \mathrm{tr}^B \hat{\rho}_R, \quad (3.49)$$

where $\hat{\rho}_R = \hat{P}_R/d_R$, $\hat{P}_R$ is the projector onto $\mathcal{H}^R$ and d_R its dimension. This allows

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us to rewrite the last equation in the spirit of (3.1) as

$$\text{Typ}(\psi : \text{tr}^B |\psi\rangle\langle\psi| \approx \text{tr}^B \hat{\rho}_R). \quad (3.50)$$

In particular for $\mathcal{H}^R = \mathcal{H}_{\text{mc}}$, the micro-canonical energy shell, and suitable self-adjoint operators $\hat{A}$ on $\mathcal{H}$ typical wave functions $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ are such that they yield the same statistics for the outcomes of experiments as the micro-canonical density matrix $\hat{\rho}_{\text{mc}}$. In other words ensembles are explained via typicality (see Section 11.1).

Second, it allows us to make sense of the distribution of wave functions for subsystems in thermal equilibrium via so called GAP measures (for details see Part III and Appendix 11.2). Such a wave function is defined along the lines of the conditional wave function in BM and we denote it here as $\psi^S \in \mathbb{S}(\mathcal{H}^S)$. It's a random element and the typical distribution is the GAP-measure: more precisely, let S and B be weakly coupled and B large enough. Then for most ONBs of $\mathcal{H}^B$ and most $\Psi \in \mathbb{S}(\mathcal{H}^S \otimes \mathcal{H}^B)$ the subsystem wave function ψ^S has the distribution $\text{GAP}_{\hat{\rho}_{\text{can}}}$. Note that this is a statement about a typical measure. As above, using (3.1),

$$\text{Typ}(\Psi, \text{ONB} : \mu_{\psi^S} \approx \text{GAP}_{\hat{\rho}_{\text{can}}}), \quad (3.51)$$

where μ_{ψ^S} denotes the usual quantum distribution of ψ^S (see below in Part III).

What the typicality results, even though posed in the standard quantum setting, show is that there is an objective way on justifying the ensembles. Further that there is a reasonable view on what ensembles mean.

Primitive Ontology

As we saw above the PO account is extremely successful in solving fundamental problems of physics, such as the measurement problem or the problem of irreversibility. That motivates the question whether there are other areas in physics where this approach might also work. With BM and BCSM (see Section 3.3.2 and Section 2.7) and their similarities in mind we try to formulate a more generic setting of the Boltzmannian framework (BF).

Based on the notion of a PO, we assign an actual state as follows:

$$s = (q, \eta) \in \mathcal{S}^\ell, \quad (3.52)$$

with state space $\mathcal{S}^\ell = \mathcal{Q} \times \mathcal{E}$ (the state space might have some constraints due to conservation laws or symmetries. But we will not be bothered with this here). Examples are for instance Bohmian mechanics, where $s = (Q, \Psi)$ with particle configurations Q and wave function Ψ or classical mechanics where $s = (x, p)$ with particle positions x and particle momenta p . In general $q \in \mathcal{Q}$, with configuration space $\mathcal{Q}$, denotes the PO part and $\eta \in \mathcal{E}$ is also part of the ontology, but not the PO. η can be thought

of as descendants of q such as momenta or velocities in classical mechanics or as an object guiding the PO³⁷, such as the universal wave function in Bohmian mechanics (see Section 3.3.2).

The idea that basic entities build up the macro world is related to scientific practice, as Einstein put it, might just be “a refinement of everyday thinking”[89, p.349]. A more philosophical presentation of that statement is the one between the manifest image and the scientific image, which together build up the overall view of the world we experience [246] and its application to physics [194]. The manifest image is the world of our everyday experience made up of macroscopic objects, such as tables, chairs, trees and so on. The scientific image is a world consisting of theoretical objects, such as superstrings, atoms or gravitational waves. With this in mind, one can understand the following characterization of statistical physics by Spohn and Lebowitz, which to them

”[...] is the bridge between world of the atom and the world of the object. Man lives in the latter world but wishes, for aesthetic as well as for practical reasons, to understand the relation between the two worlds. This is the task of statistical mechanics.”[257, p.109]

The PO proposal does just that as it consists of elements in three-dimensional space $\mathbb{R}^3$ (or space-time). This allows to compare the macroscopically observed motion with the motion of the PO [6]. That is there is an epistemic reason to rely on the PO account. It relates to empirical facts and is robust in testing these [172]. This can be done by appealing to explanatory schemes. Properties of physical objects can be explained by appealing to the behavior of the PO [5]. This can be related to classical mechanics, where point particles should explain the behavior of macroscopic properties, such as pressure or temperature. It can also be in terms of quantum mechanics. More general one can think of two levels of description, a lower level L_ℓ and a higher level L_h . The lower level theory, which contains the PO should properly describe the higher level.

As mentioned there are also elements which are not part of the PO, which are needed to “tell q how to move”. These are the laws to which we come next.

Remark 3.4.1. With respect to quantum mechanics one might be inclined to say that the view above is way too naive. Why should the way we think “classically”, that is in terms of scientific and manifest image, also be valid in the quantum realm? Famously this has been pointed out by Heisenberg

“the idea of an objective real world whose smallest parts exist objectively in the same sense as stones or trees exist, independently of whether or not we observe them ... is impossible ...”[118, p.2]

³⁷Note that with $\mathcal{L}$ we do not mean the Schrödinger equation or the Hamilton equation.

and further

“We can now longer speak of the behavior of the particle independently of the process of observation. As a final consequence, the natural laws formulated mathematically in quantum theory no longer deal with the elementary particles themselves but with our knowledge of them. Nor is it any longer possible to ask whether or not these particles exist in space and time objectively.”[118, p.2]

We reject this view. There is a way to talk objectively about the world. That is why the PO proposal has been established. As in “quantum theories without observers”, such as BM or GRW³⁸ collapse models [118]. These are quantum theories, which solve the measurement problem [172, 97]. These theories have a well posed PO, which describes matter in space and time (see [6] for more details). GRW and BM have a dual structure (PO, Ψ) the PO “providing the decoration” and the wave function Ψ governing the PO [6]; for the PO proposals in GRW theories see [6, Sec.4] or [287, Sec.3.3.4]. $\diamond$

Laws of a Theory

The laws of a theory are among the non-primitive variables [5]. They tell the matter how to move. What we have in mind here (and try to build upon) are BM and Hamiltonian mechanics, where the equations of motion for Q and X are given in terms of an ordinary differential equation (ODE)

$$\dot{X} = \mathbf{v}^H(X) \quad (3.53)$$

$$\dot{Q} = \mathbf{v}^\Psi(Q), \quad (3.54)$$

such that their solutions are given by the respective flows. Now in BM one first has to solve the Schrödinger equation for Ψ in order to use its solution to determine the evolution of $Q(t)$. Here Ψ and H govern or generate the dynamics.

Let us generalize this. Let $s \in \mathcal{S}^\ell$ and let $\mathcal{L}$ denote the “law”. The most simple way to write down a law might look as follows

$$\dot{s}(t) = \mathcal{L}(s(t)). \quad (3.55)$$

Here $\mathcal{L}(s(t))$ means that the law “acts on” or governs $s \in \mathcal{S}^\ell$. We use this rough notation and mention that there is also the possibility that the time evolution of q is given in terms of η . Laws can look differently, say e.g., $\dot{q} = \mathcal{L}(\eta)$ or $\dot{s} = \mathcal{L}(s)$. But we think of them simply as in (3.55).

In cases such as (3.53), vector fields are defined on the respective state spaces. We will consider such evolutions here. That means $\mathcal{L}$ defines a vector field on $\mathcal{S}^\ell$, whose

³⁸Short for Ghirardi-Rimini-Weber.

integral curves are the possible evolutions of $s(t)$. As a solution to (3.55) is given by the flow $\Phi_{t,t_0} : \mathcal{S}^\ell \rightarrow \mathcal{S}^\ell$, such that

$$s(t) = \Phi_{t,t_0}^{\mathcal{L}}(s_0) \quad (3.56)$$

is the unique solution of (3.55) with initial condition $s(t_0) = s_0$. There might be other possibilities for $\mathcal{L}$ as in (3.55), but these are certainly more complicated than the one just discussed (so we will not be bothered by them for the sake of our discussion here). For a proper investigation of such issues it would certainly be helpful to take considerations about the metaphysics of laws of nature into account. Depending on the theory one is considering appropriate statements regarding boundary laws might have to be formulated. We will not do this here; see [53] for more on that. Still let us make a small remark.

Remark 3.4.2. Let us comment here on a different type of law having its roots in the problem of irreversibility. Usually low entropy states are prepared, say a gas is put into one part of a box (well isolated) and then after releasing some constraint the gas will evolve such that after some time the gas particles are spatially uniformly distributed. This procedure can not be performed for the prime example of a closed system, namely the universe. In that case one has to explain the low entropy initial state of the universe. There is one proposal called the past hypothesis (PH), which can be seen as a law of nature [51]. For quantum systems it states the following (see, e.g., [55, 136, 51])

Past Hypothesis: The initial state of the universe Ψ_{t_0} is typical in $\mathcal{H}_{\nu_0}$, where the ν_0 is a low entropy macro state.

It is important to note that typicality appears in the PH. This shows the relevance of it from a different angle. So far, we discussed typicality in terms of the dynamical evolution or the typical behavior of subsystems. But here it appears in a key problem of making sense of the arrow of time, that is typicality is not only present in the dynamical laws, but also in the decisive boundary law. Note that the PH has also interesting consequences for the quantum ontology [51]. $\diamond$

Bridging Realms

Another key aspect of the success in Boltzmann's reasoning is the distinction between the microscopic and the macroscopic realm (see, e.g., [177, 170]). For instance in classical mechanics different micro states $X, X' \in \Gamma_M$ represent the same macro state M . With this in mind we try to do the following generalization.

Suppose there are two possible levels of description L_h , called the higher level and L_ℓ called the lower level. An example that comes to mind immediately is that L_h corresponds to the macroscopic observable realm, while L_ℓ corresponds to the

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microscopic realm. Here we want to keep it more generic as one could also for example think of L_h as a mesoscopic level. It's not unusual in physics that relations between two different scales are investigated to see what emerges on L_h or whether something can be reduced to L_ℓ or whether different physical effects appear at different scales.

Let us denote the state space of the higher level L_h as $\mathcal{S}^h$ and the state space of the lower level L_ℓ as $\mathcal{S}^\ell$. Let B_i , with $i \in \{1, \dots, K\}$ denote a collection of states on L_h . The micro states are as before elements of $\mathcal{S}^\ell$, that is $s \in \mathcal{S}^\ell$. Let us for simplicity consider only one state $B_1 = B$.

The aim is to connect these two levels, such that the states on the higher level L_h are expressed through the states on the lower level L_ℓ . This can be done via a *bridging procedure* connecting $\mathcal{S}^\ell$ and $\mathcal{S}^h$ in a reasonable way

$$B : \mathcal{S}^\ell \rightarrow \mathbb{R}, \quad s \mapsto B(s) \quad (3.57)$$

In particular we want states on L_ℓ describe states at L_h , in such a way that micro states have the “same look” on the L_h . We say that $s, s' \in \mathcal{S}_i^\ell$ “look the same” on L_h given that there is a *resolution*

$$R : \mathbb{R} \rightarrow \mathbb{R} \quad (3.58)$$

such that

$$B^R(s) = R(B(s)) = (R \circ B)(s). \quad (3.59)$$

That is $s, s' \in \mathcal{S}^\ell$ both represent the same state $B^R(s)$ on L_h , more precisely

$$B^R(s) = B^R(s'). \quad (3.60)$$

An example for such a procedure can look like this (same as in Section 2.7). Let $R(x) = \lceil x/\Delta x \rceil \Delta x$, where $\lceil x \rceil$ with $x \in \mathbb{R}$ denotes the next integer close to x and thus $B^R(s) = \lceil b/\Delta b \rceil \Delta b$ with $\Delta b > 0$. Here b denotes a value of $B(s)$, i.e., $B(s) = b$, such as for the Hamilton function and energy E we have $H(X) = E$. There is no general answer for choosing a resolution R . There might be a fitting one depending on the physics one is encountering.

This allows to define a partition of $\mathcal{S}^\ell$ depending on the resolution R , that is

$$\mathcal{S}^\ell = \bigcup_h \mathcal{S}_h^{R,\ell} \quad (3.61)$$

with

$$\mathcal{S}_h^{R,\ell} = \{s \in \mathcal{S}^\ell : B^R(s) = h\}. \quad (3.62)$$

One can generalize this to more macro variables B_i with $i \in \{1, \dots, K\}$ and by analogous steps finds that a partition given a resolution R reads

$$\mathcal{S}_i^{R,\ell} = \{s \in \mathcal{S}^\ell : B_i^R(s) = h_i, \forall i \in [K]\}, \quad (3.63)$$

where h_i describes the state on $\mathcal{S}^h$. A state on the higher level is then given by the tuple $h = (h_1, \dots, h_K) \in \mathcal{S}^{R,h}$. One usually refers to the resolution also as coarse-graining. Generically it's not easy to tell, which states on a lower level still represent states on a higher level and thus to choose the right partition of $\mathcal{S}^{R,\ell}$. Regarding the paradigmatic case of the lower level being the microscopic realm and the higher level being the macroscopic world one can say this: although being vague in the sense whether this particular micro state represents a particular macro state and another one does not change the overall picture. There are reasonable choices as we have for instance a clear agreement on what we call a tree or a planet. Although these might be extreme examples this connects to the discussion in the beginning of this chapter about the scientific and the manifest image. It is the world we experience and its phenomena we aim to explain and that also leads us to coarse-graining procedures which account for that. That does not mean that these phenomena depend on the coarse-graining choices we make. They depend in the trivial sense on us, because that is how we experience the world and how we try to analyze the phenomena we observe (see also [169, p.15] [284, p.57]). One can also note that as soon as one sends the number of particles N to infinity more precise definitions of macro states can be made [284, p.57]. But that is not our aim here. Our goal is to find out which regularities appear on the higher level based on the fact that most states on the lower level connected to the higher level yield such a typical behavior. To this end we need to find a measure, which tells us what most with respect to the higher level means. We will do so now.

Typicality Analysis

A typicality analysis is the proper way to explain emergent behavior on a higher level from an underlying lower level³⁹. As we have seen this can depend on a PO (typicality results from quantum statistical mechanics provide an explanation for thermal behaviour they do not rely on a PO), the laws governing it and a bridging procedure between the lower and the higher level. What we still need is a typicality measure in order to make such statements.

With (3.1) in mind we say what it means for our setting so far. A property P is typical within $\mathcal{S}^\ell$ if almost all elements of $\mathcal{S}^\ell$ instantiate P . In order to make this more precise we need to define a measure. We can not give a general answer here, besides the fact that the measure should not change under time evolution (for further criteria see [169, Sec.6.2]). Motivated by the fact that for classical systems (see Section 2.7) and Bohmian mechanics (see Section 3.3.2 and [169, 84]) the measure is related to the entity that governs the PO, we assume that such a measure is given through $\mathcal{L}$ and

³⁹For a discussion on how explanations in the philosophy of science context enter and are related to typicality see [305]

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denote is has $\mu_{\mathcal{L}}$, such that $\mu_{\mathcal{L}}(\mathcal{S}^\ell) = 1$ (we are not concerned here about precise measure theoretic notions). That means a phenomenon or property P on a higher level is typical if

$$\mu_{\mathcal{L}}\{s \in \mathcal{S}^\ell : P(s)\} \approx \mu_{\mathcal{L}}(\mathcal{S}^\ell). \quad (3.64)$$

That is, the question is whether one can find a dominant subset of $\mathcal{S}^\ell$ that has by far the largest measure and thus yields typical emergent behavior on a higher level.

We have seen for both BM and BCSM that typicality measures related empirical distributions with theoretical distributions. That is the typicality measure connects the actual state of the PO with a theoretical distribution; note that regarding actuality this makes also sense from the point of view of wave functions. That aside we generalize the typicality statements about the Maxwell Boltzmann distribution and the quantum equilibrium distribution as follows. Let $s \in \mathcal{S}^\ell$ and let $\mu_{\text{emp}}(s)$ denote the empirical distribution and let $\mu_{\text{th}}(s)$ denote the theoretical distribution. Statements we would be interested in for other theories than, for instance BM or BCSM containing a PO would be of the form

$$\mu_{\mathcal{L}}(\{s : |\mu_{\text{emp}}(s) - \mu_{\text{th}}(s)| < \varepsilon\}) \approx 1 \quad (3.65)$$

in a suitable, say “macroscopic” or “higher level” limit and for any $\varepsilon > 0$.

It would be of interest to consider examples. Some that come to mind from condensed matter physics, where two separate levels of description are used and the higher level properties emerge in a large particle number limit are Bose-Einstein condensation [99] and Ginzburg-Landau theory, which is a phenomenological theory for superconductivity without relying on microscopic details.

Part II.

Second Law in Boltzmannian Quantum Framework

4. Motivation and Problems

As mentioned in the beginning (see Part I) understanding the emergence of macroscopic behavior from an underlying microscopic theory is one of the main aims of statistical mechanics. Most famously this aim has been investigated for the laws of thermodynamics, especially the second law (and also the minus first law). We have seen in the last part of this thesis that the minus first law can be coherently understood within the BQF. This motivates the question, whether the same can be done for the second law. We will show in this part that this is indeed the case as we present several novel formulations for the second law. While two of these are agnostic with respect to the measurement problem, we also propose a more fundamentally sound version of the second law appealing to Bohmian mechanics (BM).

Let us begin with the central quantity for the second law: entropy and discuss its status in Section 4.1. Afterwards in Section 4.2 we elaborate why we expect entropy to increase after all. We end in Section 4.3 with comparing different notions of entropy in quantum mechanics, highlighting the quantum Boltzmann entropy.

4.1. Status of Second Law

Explaining the second law of thermodynamics from the underlying microscopic dynamics is a long standing problem in physics. From the times of kinetic theory [27, 28, 46], to the early days of quantum mechanics [205, 208] all the way until today [198, 262, 270, 122, 136]. As it is clearly not possible to discuss all of the approaches taken, we only focus on some of them relevant for our context.

Classically, the second law of thermodynamics is related to the famous H-theorem of Ludwig Boltzmann and is directly connected to the Boltzmann equation [27, 28]; see also [121] and [170, 165] for a modern discussion. The classical Gibbs entropy has not much to say here, as it remains constant as time evolves. A fact that can be easily seen following from Liouville's theorem. As the Hamiltonian flow (see Section 2.7) preserves volumes in phase space, it follows that [136, p.6]

$$S_G(\rho \circ \Phi_{-t}) = S_G(\rho) \quad (4.1)$$

where

$$S_G(\rho) = -k_B \int_{\Gamma} dx \, \rho(x) \log \rho(x). \quad (4.2)$$

Different proposals have been made to talk reasonably about the Gibbs entropy as *the* entropy also allowing it to increase. Such proposals try to argue for different evolution laws or claimed that Clausius' version of the second law is not correct [136, Sec.8].

A quantum analog of the H-theorem has been proposed by von Neumann [205], but as we discussed above in Section 2.5 it is actually not an analog and thus not lead to an understanding of entropy increase.

Pauli [208] aimed at a quantum mechanical derivation of the second law taking both individualist and ensemblistic viewpoints, acutally making three proposals [136]. Pauli's reasoning makes use of a master equation and the repeated randomness assumption (see, e.g., [202]); for details see [281, Chap. XII], [151, Chap.VI] or [238].

We follow and build on a conjecture stated in [136]:

Conjecture: In Bohmian mechanics and collapse theories, for macroscopic systems $\mathcal{S}$ with reasonable Hamiltonian $\hat{H}$ and decomposition $\mathcal{H} = \bigoplus_{\nu} \mathcal{H}_{\nu}$, every ν' and most $\psi \in \mathbb{S}(\mathcal{H}_{\nu'})$ are such that with probability close to one, $S_{\text{QB}}(\mathcal{S})$ is non-decreasing with time, except for infrequent, shallow, and short lived valleys, until it reaches the thermal equilibrium value. Moreover, after reaching that value, $S_{\text{QB}}(\mathcal{S})$ stays at that value for a very long time.

We will elaborate on the details of this conjecture below. Let us at least say this: the conjecture has been stated with an eye on solving the measurement problem, a point we dwell on in Section 3.3.1. Further, since the goal is to explain the emergence of the second law, a reasonable choice of the Hamiltonian $\hat{H}$ means to choose a generic $\hat{H}$, instead of a particular model. This is valid as entropy increase is a robust phenomena, not depending to much on the exact microscopics of a system; an example for a generic $\hat{H}$ is a random matrix (see Section 2.3). We expect entropy increase with time, except for infrequent, shallow, and short lived valleys. To make this more precise we need a quantity, which expresses how much the behavior is violated. This will be done below. Certainly due to Poincaré recurrence, entropy will not stay at its maximal value for all times, but certainly for long times. Recurrence times, at least classically grow with the number of particles [58]. For closed quantum systems similar statement are expected to hold [202].

In particular we will explain now how $S_{\text{QB}}(\mathcal{S})$ is defined and why we can expect it as a good notion of entropy relevant for the second law.

4.2. Reasons to Expect Increase of Quantum Boltzmann Entropy

We now define and give some reasons, why we expect entropy to increase.

Thermalization: As discussed in Part I a pure state ψ_t (under the evolution of a random Hamiltonian) will sooner or later be very close to $\mathcal{H}_{\text{eq}}$ for an overwhelmingly long time. Thus, if thermalization occurs, one should also expect entropy to increase⁴⁰.

The conceptual idea of increasing entropy in the BQF is quite natural and in spirit similar to the classical setting [136]. See (4.13) for the definition of the quantum Boltzmann entropy (unfortunately we have to anticipate the definition). Recalling that the energy shell is decomposed into subspaces

$$\mathcal{H}_{\text{mc}} = \bigoplus_{\nu} \mathcal{H}_{\nu}, \quad (4.3)$$

the unitary time evolution carries an initial state $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$ through different subspaces, in such a way that

$$\text{if } e^{-i\hat{H}t} \mathcal{H}_{\nu_0} \subseteq \mathcal{H}_{\nu}, \text{ then } S_{\text{QB}}(\nu) \geq S_{\text{QB}}(\nu_0), \quad (4.4)$$

ultimately reaching its maximal equilibrium value $S_{\text{QB}}(\text{eq})$; here $\nu = \text{eq}$ denotes the thermal equilibrium macro state.

Now $S_{\text{QB}}(\nu)$ is not explicitly time dependent. Thus one has to say what it actually means that

$$S_{\text{QB}}(\nu) = k_{\text{B}} \log d_{\nu} \quad (4.5)$$

increases with time. Another point worth mentioning here is that in general a wave function $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ can be in a superposition with contributions from different $\mathcal{H}_{\nu}$'s. Hence we have to specify what it means for a wave function to “lie” and “go through” a certain subspace. Well that turns out to be not too hard, as one can consider the macroscopic superpositions weights

$$p_{\nu}(t) = \|\hat{P}_{\nu}\psi_t\|^2, \quad (4.6)$$

which serve that purpose; note that we will use $p_{\nu}(t)$ and $\|\hat{P}_{\nu}\psi_t\|^2$ interchangeably. We will use these below in Section 5.1 to explain entropy increase.

But for now let us give some further reasons why looking for an explanation of the second law in the BQF is promising.

Classical analog: The second law in the BQF serves as an analogy to the classical case (see 2.7). Just as in classical mechanics macro sets Γ_{ν} have vastly different

⁴⁰For the distinction between the minus first and second law see [36, 149] and the cited references therein. Roughly the idea is that according to the minus first law a closed system sooner or later reaches thermal equilibrium. The second law states that entropy for a closed system never decreases. The difference might be that along the evolution, entropy does not increase all the time, but the system will still thermalize sooner or later.

volumes, the quantum macro spaces $\mathcal{H}_\nu$ have vastly different dimensions. As phase space volume is conserved classically, the dimension (of subspaces) is conserved under the unitary Schrödinger evolution. Goldstein and Lebowitz [129] discuss certain traits of the classical Boltzmann entropy in non-equilibrium. These ideas carry on to the quantum realm [9, Sec. 7.2.5]. Suppose a macro state $\nu(t)$ evolves autonomously according to some evolution equation (e.g. some hydrodynamic equation or the Boltzmann equation). This means that on a micro level the macro evolution from $\nu(t_1)$ to $\nu(t_2)$ (with $t_2 \geq t_1$) is such that the unitary operator $\hat{U}_{t_2-t_1}$ “shoves” $\mathcal{H}_{\nu(t_1)}$ to $\mathcal{H}_{\nu(t_2)}$. That immediately implies that entropy has increased: $S_B(\nu(t_2)) \geq S_B(\nu(t_1))$ (compare with (4.4) and note that S_B is the classical Boltzmann entropy (2.65)).

Normal typicality: We have seen above in Section 2.5 that the typical evolution of (4.6) is deterministic approaching a certain value (depending on the case) which is constant and depends on the subspaces involved. That leads us to believe that these long time limit values have something to do with the second law. Especially as by dominance of thermal equilibrium, there is one subspace for which $d_{\text{eq}}/d \approx 1$ and thus the entropy of this state is the maximal entropy. Although that is not the end of the story.

Two times: Consider at least two macrostates ν and ν' with vastly different dimensions: let $\hat{H}$ and $t \neq 0$ be arbitrary but fixed [136, Prop.1]. If $d_{\nu'} \ll d_\nu$, then for most $\psi_0 \in \mathbb{S}(\mathcal{H}_\nu)$:

$$\|P_{\nu'}\psi_t\|^2 \ll 1. \quad (4.7)$$

In terms of entropy this means that if $S_{\text{QB}}(\nu')$ is less than $S_{\text{QB}}(\nu)$, then for most initial states the time evolution is such that S_{QB} will not decrease or in other words: ψ_t will evolve such that it will not be close to $\mathcal{H}_{\nu'}$ anymore.

Note that here only two instances in time were considered, but *not* the entire history of the macro evolution $p_\nu(t)$. We are interested in the whole time evolution.

Simple example: A full time evolution is considered in the following simple example. Let $\mathcal{H}_{\text{mc}} = \mathcal{H}_1 \oplus \mathcal{H}_2$ be two subspaces with dimension d_1 and $d_2 = D - 1$. Let $\hat{H} = \sum_n E_n |\phi_n\rangle\langle\phi_n|$ be the Hamiltonian. We start with $\psi_0 \in \mathbb{S}(\mathcal{H}_1)$ and ask, how much of ψ_t will be left in $\mathcal{H}_1$. Let $\psi_0 = \sum_n c_n |\phi_n\rangle$ and assume that the c_n are uniformly distributed with variance $1/D$; meaning the direction of $\mathcal{H}_1$ is chosen randomly. Since the energy levels are very close, we have for large D

$$\langle\psi_0|\psi_t\rangle \approx \frac{1}{D} \sum_n e^{-itE_n} \approx \int_{\mathbb{R}} dE \rho(E) e^{-itE} = \tilde{\rho}(t) \quad (4.8)$$

which is (up to a factor) the Fourier transform $\tilde{\rho}(t)$ of the density of states $\rho(E)$; the observation that the Fourier transform plays a key role in the temporal evolution of a system with many degrees of freedom has also been made by Reimann [223]. If $\hat{P}_1$

is the projector on $\mathcal{H}_1$, then

$$||\hat{P}_1\psi_t||^2 = |\langle\psi_0|\psi_t\rangle|^2 \approx |\tilde{\rho}(t)|^2. \quad (4.9)$$

The Riemann-Lebesgue lemma implies that ψ_t will completely evolve into the bigger subspace as long as our approximation is valid. Therefore entropy increases. This is not in conflict with the Poincaré recurrence theorem, as the phases on the left hand side of (4.8) disappear on the right hand side.

Up to now it has been left open how exactly $\rho(E)$ looks like. Assume for instance that $\hat{H}$ is a random matrix (see Section 6.2 for another choice). Then, for fairly standard random matrix ensembles such as the Gaussian unitary ensemble, $\rho(E) = (1/2\pi)\sqrt{4 - E^2}$ is the semi-circle density (see Section 6.2 or [302, 64]). Thus

$$||\hat{P}_1\psi_t||^2 \approx \frac{J_1^2(2t)}{t^2} \quad (4.10)$$

with $J_1(x)$ being the Bessel function of first kind. Due to the monotonicity properties of $(J_1(2t)/t)^2$ (see Figure 6.1), the weights $||\hat{P}_1\psi_t||^2$ are “more or less” decreasing and the evolution will be such that ψ_t for $t > 0$ will lie in the larger subspace, which is the thermal equilibrium subspace.

Numerics: Numerical simulations of a simple setup (with four subspaces) in [277] suggest that for a randomly chosen Hamiltonian, the evolution of the macroscopic weights is such that they show thermal behavior (see figure 4.1). Let us just comment briefly and refer the reader to the cited reference. The choice of the Hamiltonian is different to the one used in [131, 135].

4.3. Quantum Entropy

We will now discuss why we use the quantum Boltzmann entropy. Our main emphasis lies on the fact that among other proposals of entropy it does not rely on the performance of measurements or the knowledge of observers. A system does have a quantum Boltzmann entropy and it does align with the properties of macroscopic thermodynamic entropy. In particular it allows to properly formulate a second law.

Before we start, here’s an anecdote. According to [282, p.180], Shannon when trying to find a name for his nowadays well known entropy formula, said:

“My greatest concern was what to call it. I thought of calling it ‘information,’ but the word was overly used, so I decided to call it ‘uncertainty.’ When I discussed it with John von Neumann, he had a better idea. Von Neumann told me, ‘You should call it entropy, for two reasons. In the first place your uncertainty function has been used in statistical mechanics under that name, so it already has a name. In the second place, and more important, no one knows what entropy really is, so in a debate you will always have the advantage.’ ”

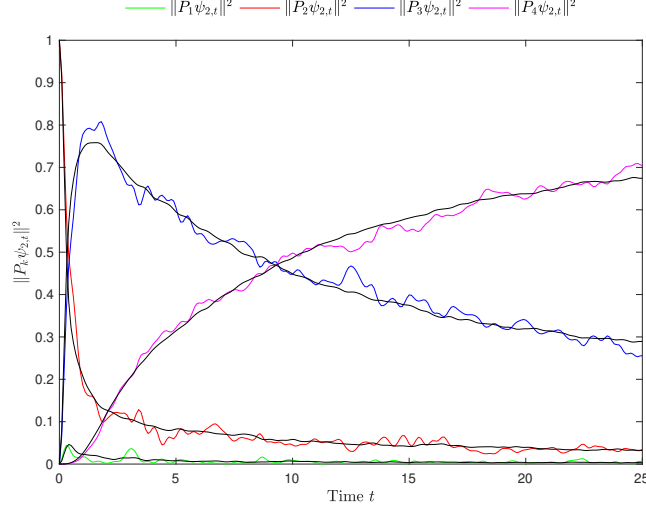


Figure 4.1.: Example of time evolution of superposition weights $\|\hat{P}_\nu \psi_t\|^2$, here in a Hilbert space of dimension $D = 2222$ decomposed into four macrospace with dimension $d_1 = 2, d_2 = 20, d_3 = 200$ and $d_4 = 2000$ from [277]. The initial state is chosen randomly from $\mathbb{S}(\mathcal{H}_2)$. The evolution is such that $\|\hat{P}_4 \psi_t\|^2$ after some time t is larger than the other weights. For more details see [277].

Let us comment on that: the last point von Neumann made, of having an edge regarding entropy in any ways, is either meant as a joke or shows how serious the issue is. We will see that one can pin down the right entropy relevant for the second law: Boltzmann's entropy. The first point of von Neumann will be considered below, as its a common mismoner leading to wrong conclusions about the right notion of entropy.

Bridging Entropy

Before we discuss some of the entropies heavily used in quantum statistical mechanics, we should make clear what entropy has to account for. The main aim is to derive the second law from the microscopic dynamics. So in some sense the entropies have to be related and have to share the same properties [129]. In particular the microscopic entropy has to have the properties of thermodynamic entropy, which we also denote as the Clausius entropy S_C . Clausius was the first to formulate the increase of entropy as a law. A further property of S_C is that it's extensive, meaning that for two systems A and B with entropy S_C^A and S_C^B being connected after isolation, the total entropy

of $A \cup B$ reads

$$S_C^{A \cup B} = S_C^A + S_C^B. \quad (4.11)$$

Further it has to connect the microscopic realm with the macroscopic realm. This has been a key insight of Ludwig Boltzmann [9, 169, 177]. For classical systems this first means that a phase point describing the state of an individual system, say a glass of water, is assigned an entropy value. More precisely, it means that a several different phase points all having the same “macroscopic look” can have the same entropy value. That is for $X \in \Gamma_\nu$ the (classical) Boltzmann entropy reads

$$S_B(X) = k_B \log \text{vol}(\Gamma_\nu). \quad (4.12)$$

It can easily be seen that it has the properties (basically through the properties of the logarithm) of the Clausius entropy S_C and also has the possibility to increase as we will see below. This can be made very precise although there have been not much instances where it has been shown rigorously.

Let us end with a conceptual note. As for thermalization we take the individualist view that phase points and pure states yield thermal behavior. Our guiding thought here is that our knowledge about a system does not matter what the value of the macroscopic entropy is. It does not matter whether the entropy of the system is measured or not. There is simply a fact whether a cup of coffee or the universe has a certain entropy value or whether its in thermal equilibrium or not (clearly that is not the case for the earth or the universe). Thereby we appeal to typicality as before. Thermal equilibrium is typical, as well as the approach to thermal equilibrium is typical and finally also the increase of entropy is typical.

Quantum Boltzmann Entropy

The **quantum Boltzmann entropy** is defined analogously to classical mechanics (see Section 2.7). The role of phase space volume for a region Γ_ν in phase space is now played by the dimension d_ν of the subspace $\mathcal{H}_\nu$. A proposal that has first been given by Lebowitz [177] in 2008, while a similar formula was given by Griffiths in 1994 (see [139], p.153). For $\psi \in \mathbb{S}(\mathcal{H}_\nu)$, it reads [135]:

$$S_{QB}(\psi) = k_B \log \dim \mathcal{H}_\nu. \quad (4.13)$$

Interesting to mention is that Einstein [88] came up with a proposal for the entropy in quantum mechanics, which is similar in spirit to that of Boltzmann. He [88, Eq.4a] argued that for a macro state one should assign the entropy to be proportional to the logarithm of the “number of elementary quantum states” [88, p.36], which are representing this specific macro state.

Before we state its properties let us mention that underlying all these properties

is the fact that macro and micro realm are *bridged*, a key insight of Boltzmann (see, e.g., [170, 9]). With that in mind, here are the properties of (4.13) [136]⁴¹.

It is defined on the *individual* microstates ψ , that represent the macro state ν . This means that it connects the microscopic dynamics with the macroscopic dynamics.

The quantum Boltzmann entropy (4.13) is also defined out of equilibrium. An initial state ψ that starts out in some non-equilibrium subspace $\mathcal{H}_\nu$ evolves unitarily. Thereby moving through different subspaces changing its subspace and therefore its entropy. Thus leaving the chance to be in line with the second law of thermodynamics⁴²

As (4.13) connects micro and macro realm it should also fulfill the properties of the thermodynamic entropy. One of them is extensivity. Consider a closed system $\mathcal{S}$ consisting of two subsystems $\mathcal{S}_1$ and $\mathcal{S}_2$, such that $\mathcal{S} = \mathcal{S}_1 \cup \mathcal{S}_2$. Let $\mathcal{H}_1 = \bigoplus_{\nu_1} \mathcal{H}_{\nu_1}$ and $\mathcal{H}_2 = \bigoplus_{\nu_2} \mathcal{H}_{\nu_2}$ be their respective subspaces. If $\mathcal{S}_1$ and $\mathcal{S}_2$ interact weakly, then

$$\mathcal{H}_1 \otimes \mathcal{H}_2 = \bigoplus_{\nu_1, \nu_2} \mathcal{H}_{\nu_1} \otimes \mathcal{H}_{\nu_2} \quad (4.14)$$

is the Hilbert space of $\mathcal{S}$. It follows that the entropy of the macrostate for the composed system (ν_1, ν_2) is given by

$$S_{\text{QB}}(\nu_1, \nu_2) = S_{\text{QB}}(\nu_1) + S_{\text{QB}}(\nu_2), \quad (4.15)$$

and thus fulfilling the property of the thermodynamic entropy being an extensive quantity.

As a consequence of dominance of thermal equilibrium, i.e. $d_{\text{eq}}/D \approx 1$, one has that

$$S_{\text{QB}}(\text{eq}) \approx k_B \log \dim \mathcal{H}_{\text{mc}} = S_C(E), \quad (4.16)$$

which is the thermodynamic entropy in thermal equilibrium.

Let us in the end just briefly mention that Tasaki has a related view to ours regarding the definition of entropy for closed quantum systems [272, Sec. 5].

Remark 4.3.1. In our discussion we focused on closed systems. Clearly most systems interact with their environment. So it would be of interest to see how the BQF changes with respect to that. Considerations in this direction have been made in [136]. That might also shed a perspective on recent research on open systems (see, e.g., [231, 70]). $\diamond$

⁴¹The order does not mean that one of them is more important than the other.

⁴²Although the state will have several contributions in several subspaces, due to superposition; a problem that we'll deal with later.

Quantum Gibbs Entropy

Here is the most common notion of entropy in quantum mechanics: the von Neumann entropy. There is actually another notion of entropy that was proposed by von Neumann [205], nowadays known as observational entropy [236, 235], which will be discussed below. That is why one might refer to these types of entropies as quantum Gibbs entropies.

For a density matrix $\hat{\rho}$ on $\mathcal{H}$ the **von Neumann entropy** is defined as follows

$$S_{\text{vN}}(\hat{\rho}) = -k_{\text{B}} \operatorname{tr}(\hat{\rho} \log \hat{\rho}). \quad (4.17)$$

It is well known that (4.17) is not relevant for the second law of thermodynamics as it can not account for the non-trivial aspects of the second law since it is constant over time. Let $\hat{\rho}_t = \hat{U}_t^* \hat{\rho}_0 \hat{U}_t$ with initial state $\hat{\rho}_0$ and $\hat{U}_t = \exp(-i\hat{H}t)$, then

$$S_{\text{vN}}(\hat{\rho}_t) = -k_{\text{B}} \operatorname{tr} \left(U_t^\dagger \hat{\rho}_0 U_t \log \left(U_t^\dagger \hat{\rho}_0 U_t \right) \right) \quad (4.18)$$

$$= -k_{\text{B}} \operatorname{tr} \left(U_t^\dagger \hat{\rho}_0 U_t U_t^\dagger \log (\hat{\rho}_0) U_t \right) \quad (4.19)$$

$$= S_{\text{vN}}(\hat{\rho}_0), \quad (4.20)$$

using functional calculus⁴³ and cyclicity of the trace. Note that the same is also true for classical systems, as the Liouville theorem implies that the Gibbs entropy stays constant over time.

In thermal equilibrium the von Neumann entropy coincides with the thermodynamic entropy as well as with the quantum Boltzmann entropy, that is let $\hat{\rho}_{\text{mc}} = \hat{P}_{\text{mc}}/D$ be the micro-canonical density matrix (see Section 9.2), it immediately follows that

$$S_{\text{vN}}(\hat{\rho}_{\text{mc}}) = k_{\text{B}} \log \dim \mathcal{H}_{\text{mc}} = S_{\text{C}}(E). \quad (4.21)$$

There is another notion of entropy, called **observational entropy** that has been proposed recently and by Šafránek et al. [236, 235, 262], connecting parts of Gibbs entropy and parts of Boltzmann entropy. Von Neumann [297] wrote down a different formula for the entropy, than the one that is usually connected with him, namely (4.17). The reason for that is:

”[t]he expressions for entropy [of the form $-k \operatorname{tr} \rho \log \rho$] are not applicable here in the way they were intended, as they were computed from the perspective of an observer who can carry out all measurements that are possible in principle—i.e., regardless of whether they are macroscopic[.]”[136, p.41]

⁴³Recall that for a self-adjoint operator $\hat{A}$ with spectral decomposition $\hat{A} = \sum_{\alpha} \alpha \hat{P}_{\alpha}$ one can define $f(\hat{A}) = \sum_{\alpha} f(\alpha) \hat{P}_{\alpha}$.

As pointed out in [136] a mix of an ensemblistic as well as individualistic attitude is present.

Let us introduce the observational entropy; we follow [236]. A systems state is given by a density matrix $\hat{\rho}$ on Hilbert space $\mathcal{H}$ with $D = \dim \mathcal{H}$. Macro states are defined by the set of projectors $\{\hat{P}_i\}$, where each element $\hat{P}_i$ corresponds to a measurement outcome i . They decompose $\mathcal{H}$ into orthogonal subspaces where each subspace is the eigenspace of $\hat{P}_i$,

$$\mathcal{H} = \bigoplus_i \mathcal{H}_i. \quad (4.22)$$

Further they assume that the an observer can only get insights to the system by performing a measurement “of the projector $\hat{P}_i$ ” and cannot distinguish between different states within each subspace $\mathcal{H}_i$. The consequence they draw is that each state in $\mathcal{H}_i$ is equally probable.

The observational entropy is defined as

$$S_{\text{Obs}}(\hat{\rho}) = -k_B \sum_i p_i \log \left(\frac{p_i}{d_i} \right) \quad (4.23)$$

where $p_i = \text{tr}(\hat{P}_i \hat{\rho})$ and $d_i = \text{tr} \hat{P}_i$. It is a mixture of Boltzmann entropy and Gibbs entropy

$$S_{\text{Obs}}(\hat{\rho}) = S_{\text{Sh}}(p_i) + \langle S_B(i) \rangle_{p_i} \quad (4.24)$$

where $\langle S_B(i) \rangle_{p_i}$ is the average Boltzmann entropy (we will makes this more explicit in a minute) and $S_{\text{Sh}}(p_i)$ the Shannon entropy

$$S_{\text{Sh}}(p_i) = -k_B \sum_i p_i \log p_i. \quad (4.25)$$

Looking back at the quote in the beginning of this chapter let us say that the from of the formula itself has lead to misconceptions of $S_{\text{Sh}}(p_i)$ or the quantum Gibbs entropy in general being related to thermodynamic entropy. That has to do with the fact that Boltzmann’s reasoning regarding the H-theorem used a similar looking formula for the entropy. But its compeltely different in content (see [121, 136] for a detailed discussion).

Quantum Gibbs Entropy and its Flaws

Let us now give several reasons why the quantum Gibbs entropies stated in the last section are not useful to describe the second law and entropy in general. That is related to the discussion in the first Part I about the division between ensemblistic and

individualism. It will also appear again in the last Part III. It's about the question what it means to assign as the system's state a statistical state. That is, either a probability density on phase space for classical systems or a density matrix on Hilbert space for quantum systems. Let us for simplicity start with classical mechanics and discuss the quantum case afterwards. The critics we propose apply equally, but can be easier stated for classical systems.

In the classical case $\rho(x)$ can mean several things [136, Sec.1.2]. Relevant now is the understanding that $\rho(x)$ corresponds to the degree of belief that $x = X$. That is, the reasons an observer has, to be certain enough that the actual micro state is X . Recall that the Gibbs entropy is defined as follows

$$S_G(\rho) = -k_B \int_{\Gamma} dx \rho(x) \log \rho(x). \quad (4.26)$$

With respect to the Gibbs entropy (4.26), which we recall is understood to quantify the lack of knowledge or the uncertainty an observer has (see, e.g., [11, Sec.3, Sec.4] and [136, Sec.4] and the cited references therein). For now let us follow [136, Sec.4] calling the just stated conception of entropy “subjective entropy”, for which there are at least three problems:

First, subjective entropy yields wrong thermodynamic values [136, Sec. 4.1]. This is simply due to the fact that knowing nothing about a system does not mean that each outcome is equally likely. Goldstein et al. [136] give the following example. Suppose an isolated room contains a heater. You do not know whether the heater is on or off. If it's on, then after, say ten minutes, the entropy of the room has a value S_3 . If it's off, the value of the room has a lower entropy value $S_2 < S_3$. Regarding our ignorance we might be inclined to say that there's a chance of 50% that the heater is on and a chance of 50% that the heater is off. After ten minutes the distribution ρ evolved into regions in phase space, which differ in their macroscopic look. As a consequence the Gibbs entropy will have a value somewhere in between S_1 and S_3 . That is wrong as there is a *fact* of whether the heater was on or off yielding the corresponding thermodynamic entropy values.

Here's another similar example: suppose your office mates made tea for you. While they were preparing the tea you were in the library. You come back after some time (not knowing about the tea) and there's a cup of tea on your desk. You are unsure whether you can drink it, because you don't know if it's still too hot and might burn your mouth. So you recall from your statistical physics class that there is a certain probability that assigns also an entropy value. And if the entropy is (sufficiently) close to its maximum, this means that you will not burn your mouth and can enjoy your tea. So would you make a reasonable guess, say with 50 percent the tea is drinkable and with 50 percent it's not-drinkable (as in the example before the respective probability densities evolve in time towards different regions in phase

space) and rely on that to drink it? Hard to believe. This example shows that with respect to our actions, we should also care about what the actual value of entropy is. Physics is not just about abstract systems.

Second, subjective entropy does neither explain nor predict thermal phenomena, such as entropy increase. The flow of heat from the hotter to the cooler does not rely on an observer and his ignorance. It is hard to doubt that there are facts in nature, which do not rely on whether they are observed or measured or anything else. Nature just does what it does. The subjective view can not predict such a behavior. With respect to the examples above, there is just a fact whether the room is warm or cold or whether the tea is drinkable or not drinkable.

A third and last aspect we briefly mention is that the Gibbs entropy roughly measures the width of a probability density ρ (just plug a Gaussian distribution into (4.26)). So it does not really care about those x on which $\rho(x)$ is concentrated. In particular if one knows the system exactly, then the Gibbs entropy (4.26) should be $-\infty$. But what would that mean? And even if a system is not known exactly doesn't that mean that there is a precise state, in other words: the system itself, i.e., nature knows in which state she is in? For further details see [136, Sec.4.3] and [174].

Similar statements can be made with respect to quantum mechanics and (4.17). Here the corresponding quantity to $\rho(x)$ is a density matrix $\hat{\rho}$ on a Hilbert space $\mathcal{H}$; also called mixed state (for more see Part III). The difference is that in quantum mechanics density matrices do not only arise from a lack of knowledge, but also as reduced density matrices. This means that for a system, say $S \cup B$, the state of S can be mixed even if $S \cup B$ is in a pure state (for more see Section 9.1). This allows to define as an entropy the so called entanglement entropy, which we will not go through here as similar issues arise (for a discussion see [136, Sec.9.3]). Let us also mention that a wave function $\psi \in \mathbb{S}(\mathcal{H})$ is not the exact analog to a phase point $X \in \Gamma$ (see [136, p.12]).

The observational entropy has similar flaws as the Gibbs entropy. First of all an ensemblist view is taken in [236, 235, 234, 262]. Second, it heavily relies on the notion of measurement and can thus not account for “objective” facts of entropy increase. Another point worth mentioning in this respect is that regarding the measurement problem no clear cut is made [234] and it's more or less left to the opinion of the reader. In [262] the observational entropy is motivated by recent experiments. They claim that the quantum Boltzmann entropy can not account for these as it's “too coarse”. It is argued that the Gibbs entropy can treat microscopic systems better and thus an interpolation between the two leads to the observational entropy. The conclusion is drawn that the “Boltzmann entropy seems to be inadequate to take into account microscopic information, which is available to us now, but was not available a hundred years ago.”[262]. We disagree. The Boltzmann entropy connects the microscopic with the macroscopic realm, that is with thermodynamic entropy. Given a suitable coarse-

graining it can account for exactly that.

Here's another point worth mentioning [136, p.41]. The formula for the observational entropy (4.23) and (4.24) are more of an average entropy. First in our notation (4.24) for a pure state $\psi \in \mathbb{S}(\mathcal{H})$ reads

$$S_{\text{Obs}}(\psi) = -k_{\text{B}} \sum_{\nu} \|\hat{P}_{\nu}\psi\|^2 \log \frac{\|\hat{P}_{\nu}\psi\|^2}{d_{\nu}} \quad (4.27)$$

$$= -k_{\text{B}} \sum_{\nu} \|\hat{P}_{\nu}\psi\|^2 \log \|\hat{P}_{\nu}\psi\|^2 + k_{\text{B}} \sum_{\nu} \|\hat{P}_{\nu}\psi\|^2 \log d_{\nu}. \quad (4.28)$$

Suppose the wave function lies in some, but not too many macro spaces. What can be seen from the equation above is that $\|\hat{P}_{\nu}\psi_t\|^2 \log \|\hat{P}_{\nu}\psi_t\|^2$ can be neglected, as $\|\hat{P}_{\nu}\psi_t\|^2 \ll 1$. Then $S(\psi)$ above is just the average. But that's not what we want. We are not interested in the average temperature of the fluid in our thermosbottle [136, p.41].

5. Second Law in Boltzmannian Quantum Framework

We now introduce two proposals for the second law of thermodynamics in the BQF building on conjecture 4.1. In Section 5.1 we propose the weak second law. And in Section 5.2 we propose the strong second law. As far as the author knows these proposals have been first introduced in [286, 289]. In particular we have to point out what it means for (4.13) to increase with time as it does not depend on time explicitly, we do so in Section 5.3.

5.1. Weak Second Law: Right Moving Distributions

In order to speak about entropy increase we take the weights $p_\nu(t)$ into account, i.e., we focus on the full macroscopic history

$$(\nu, t) \mapsto \|\hat{P}_\nu \psi_t\|^2 \quad (5.1)$$

Every $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ defines for every macro space $\mathcal{H}_\nu$ a weight $p_\nu = \|\hat{P}_\nu \psi_t\|^2$. The collection of weights for all ν then define a distribution. For a unitarily evolving state, this means that the macroscopic description of the system yields a distribution for each time t and for each $\nu \in \mathcal{N}$; recall that $\mathcal{N}$ is the set of macro states. Since we are interested in entropy increase, we consider a specific ordered set of macro spaces. We define an order on $\mathcal{N}$ by $\nu < \nu'$ if and only if $d_\nu < d_{\nu'}$. We will now make two crucial definitions: first, we say that $\tilde{p}$ **lies to the right of** p and write $p \preceq \tilde{p}$ if and only if

$$\sum_{\nu \geq \nu'} p_\nu \leq \sum_{\nu \geq \nu'} \tilde{p}_\nu \quad \forall \nu' \in \mathcal{N}. \quad (5.2)$$

Second, a family of distributions $(p(t))_{t \in [0, T]}$ is **right moving** if and only if

$$\forall t_1 \leq t_2 : p(t_1) \preceq p(t_2) \quad (5.3)$$

where $t_1, t_2 \in [0, T]$. More explicit:

$$\forall t_1 \leq t_2 : \sum_{\nu \geq \nu'} p_\nu(t_1) \leq \sum_{\nu \geq \nu'} p_\nu(t_2) \quad \forall \nu' \in \mathcal{N}. \quad (5.4)$$

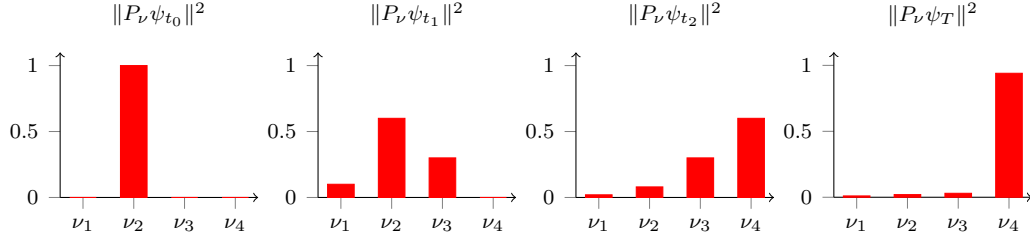


Figure 5.1.: Example of an approximately right moving distribution with four macro spaces, which illustrates the right moving behavior of the histograms. The macro spaces are ordered by dimension, i.e. ν_1 has the smallest dimension and ν_4 the largest, which means that ν_4 is the thermal equilibrium subspace. At time t_0 the system starts in ν_2 . At time t_1 the macro weights have evolved such that some part of the wavefunction evolves to the other subspaces. After time t_2 , more has evolved towards the larger subspaces ν_3 and ν_4 , than to ν_1 and ν_2 . Ultimately one ends up in the thermal equilibrium subspace $\nu_4 = \text{eq}$. The histograms are (approximately) moving to the right, towards the largest subspace.

A distribution fulfilling (5.4) is called a **right moving distribution (RMD)**.

A RMD expresses a sense of the increase of (4.13). Each $t \geq 0$ yields a histogram on the set $\mathcal{N}$ with a column for each macro state ν . As time evolves, the histogram changes and probability is transported to different macro states ν . This can be seen by the fact that the columns of each ν either shrink or rise (or possibly stay constant). The maximum entropy state is related with the largest subspace $\mathcal{H}_{\text{eq}}$. Thus for entropy to increase, probability has to be transported to larger subspaces. In our definition of $\mathcal{N}$, this means that probability has to be shoved “to the right”, which means that the columns of the histograms have (as time evolves) “move to the right”. This is what (5.4) expresses and what is also depicted in 5.1.

As stated in conjecture 4.1, the second law will be violated in exceptional cases. Probability is also transported to smaller subspaces (as can be seen in 5.1; notice however that these violations are extremely small and the small columns in 5.1 are not drawn to scale, because for realistic scenarios one would not even see them.). Compared to the transport to larger subspaces this is however negligible. Still one might want to quantify this. To phrase this in terms of RMDs, we will call these **approximately RMDs (ARMD)**. This will be made more precise below in Section 5.3.

We aim to explain entropy increase by appeal to typicality. Hence we do not aim at showing that for any initial state $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$ or/and any Hamiltonian $\hat{H}$ the macroscopic weights are right moving. Instead we focus on typical initial states or typical Hamiltonians (or even a typical decomposition); see Section 2.3 for possible choices. In general we will call such a choice a **reasonable choice**; this notion is essentially related to the reasons of why to consider typical Hamiltonians (see Section 2.3) or appealing to typicality reasoning regarding many particle systems in general (see

Section 3.1). Here and in what follows a reasonable choice refers to a typical $\hat{H}$ and/or typical $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$.

We are now able to state a version of the second law:

Weak Second Law (WSL): For a reasonable choice of $\hat{H}$, decomposition $\mathcal{H}_{\text{mc}} = \bigoplus_{\nu} \mathcal{H}_{\nu}$, initial macro state ν_0 , and $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$, the family $(p_{\nu}(t))_{t \in [0, T]}$ is an approximately RMD up to time T , where T is the time scale of reaching MATE.

An example could be to use a random Hamiltonian $\hat{H}$ with distribution $\mathbb{P}$ and a typical initial state $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$ with the consequence that typical weights with respect to $\mathbb{P}$ are given by deterministic approximations $w_{\nu}(t)$, i.e.,

$$||\hat{P}_{\nu}\psi_t||^2 \approx w_{\nu}(t). \quad (5.5)$$

The approximations $w_{\nu}(t)$ should then behave like an ARMD. We now turn to a version of the second law.

5.2. Strong Second Law: Current

Another, even stronger (see Remark 5.2.1), kind of increase of (4.13), namely via a probability current. Here, the idea is that during the time evolution of a pure state $\psi_t \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ probability is transported between different subspaces. Increase in entropy now means that there is a directedness of this transport into subspaces with larger dimension. The net current between two macrostates ν and ν' , i.e., the amount of weight transported per time from ν' to ν minus that transported from ν to ν' is defined as follows: let ν, ν' be two macro spaces and arbitrary $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$, then the (netto) current $J_{\nu\nu'}^{\psi_0}(t)$ between ν and ν' is given by

$$J_{\nu\nu'}^{\psi_0}(t) := 2\text{Im}\langle\psi_t|\hat{P}_{\nu}\hat{H}\hat{P}_{\nu'}|\psi_t\rangle \quad (5.6)$$

$$= -i\langle\psi_0|e^{i\hat{H}t}(\hat{P}_{\nu}\hat{H}\hat{P}_{\nu'} - \hat{P}_{\nu'}\hat{H}\hat{P}_{\nu})e^{-i\hat{H}t}|\psi_0\rangle. \quad (5.7)$$

The current can be derived by taking the time derivative of the weights $||\hat{P}_{\nu}\psi_t||^2$ and making use of the completeness relation $\sum_{\nu} \hat{P}_{\nu} = 1$, ultimately yielding a continuity equation:

$$\frac{d}{dt}p_{\nu}(t) = \sum_{\nu'} J_{\nu\nu'}^{\psi_0}(t). \quad (5.8)$$

From (5.8) one can see that $J_{\nu\nu'}^{\psi_0}(t)$ denotes the current from ν' to ν as the temporal change in the probability of p_{ν} is positive, that is more probability gets transported

from all the other ν 's into ν whenever all $J_{\nu\nu'}^{\psi_0}(t)$ are positive.

As for the weights moving to the right, the current does not fully “point” from subspaces with lower dimension to subspaces with higher dimension. It only does so approximately, i.e., up to violations, that in the end are negligible. Taking this into account and building on the conjecture 4.1 above, we formulate another version of the second law as follows:

Strong Second Law (SSL): For a reasonable choice of $\hat{H}$, decomposition $\mathcal{H}_{\text{mc}} = \bigoplus_{\nu} \mathcal{H}_{\nu}$, initial macro state ν_0 , and $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$, the discrete current $J_{\nu\nu'}^{\psi_0}(t)$ points overwhelmingly from smaller $\mathcal{H}_{\nu}$ to larger $\mathcal{H}_{\nu'}$:

$$J_{\nu\nu'}^{\psi_0}(t) \leq 0 \text{ for } \nu < \nu' \quad (5.9)$$

and $t \in [0, T]$, where T is the time scale of reaching MATE.

The goal is to find a reasonable setup, such that the current (5.6) typically points overwhelmingly from smaller to larger subspaces. That is, suppose for instance $\hat{H}$ and ψ_0 are sampled according to certain probability measures, say $\mathbb{P}_{\hat{H}}$ and $\mathbb{P}_{\psi_0}$, then for most $\hat{H}$ and ψ_0 with respect to these measures,

$$J_{\nu\nu'}^{\psi_0}(t) \approx C_{\nu\nu'}(t), \quad (5.10)$$

such that the deterministic approximation $C_{\nu\nu'}(t)$ points overwhelmingly from smaller $\mathcal{H}_{\nu}$ to larger $\mathcal{H}_{\nu'}$.

Remark 5.2.1 (WSL and SSL). Let us discuss the connection between the WSL and the SSL. The WSL follows from the SSL, but the SSL does not follow from the WSL. The key idea is the following: the SSL requires the current $J_{\nu\nu'}^{\psi_0}(t)$ to flow from smaller subspaces to larger subspaces. This has to hold for any pair (ν, ν') involved. In this way it is more “local” as the WSL, since it only cares about the “macroscopic” portion of probability being transported to larger subspaces, but does not care so much about individual transitions between two “neighbouring” subspaces.

The WSL is a consequence of the SSL: the SSL states that the probability (per unit time interval) flows *for each* pair (ν, ν') from smaller to larger subspaces. If this is the case, then also the weights $p_{\nu}(t)$ increase for larger subspaces, i.e., they are moving to the right and therefore fulfill the WSL.

Here’s why the WSL does not imply the SSL: the WSL is a macroscopic statement about the weights. The temporal evolution of the weights is given by the continuity equation (5.8) and thus connected with the current. The SSL states that for each pair of subspaces (ν, ν') with $\nu < \nu'$: $J_{\nu\nu'}^{\psi_0}(t) \leq 0$. This is the reason why the WSL does not follow from the SSL. Let us explain: let $L = \#\mathcal{N}$ denote the number of macro state. (5.8) yields $L - 1$ independent equations since we have the constraint

$\sum_{\nu \in \mathcal{N}} p_\nu(t) = 1$. However, at the same time it yields, $L(L-1)/2$ independent currents $J_{\nu\nu'}^{\psi_0}(t)$ (since $J_{\nu\nu'}^{\psi_0}(t) = -J_{\nu'\nu}^{\psi_0}(t)$) and thus more currents (unknown variables) than equations. This implies that even if the weights are right moving, there can still be pairs of subspaces for which the current is flowing to smaller subspaces.

Let us illustrate this with a simple example: let $\mathcal{H}_{\text{mc}} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3$, i.e., $L = 3$. It follows from (5.8), using $J_{\nu\nu'}^{\psi_0}(t) = -J_{\nu'\nu}^{\psi_0}(t)$, that

$$\frac{d}{dt}p_1(t) = J_{12}^{\psi_0}(t) + J_{13}^{\psi_0}(t), \quad (5.11)$$

$$\frac{d}{dt}p_2(t) = -J_{12}^{\psi_0}(t) + J_{23}^{\psi_0}(t), \quad (5.12)$$

$$\frac{d}{dt}p_3(t) = -J_{13}^{\psi_0}(t) - J_{23}^{\psi_0}(t). \quad (5.13)$$

We have $3(3-1)/2 = 3$ independent currents and 3 weights with the constraint $p_1(t) + p_2(t) + p_3(t) = 1$. Now let $t_1 \leq t_2$ and consider some exemplaric values for the weights, say $p_1(t_1) = 0.5, p_2(t_1) = 0.4, p_3(t_1) = 0.1$ and $p_1(t_2) = 0.2, p_2(t_2) = 0.3, p_3(t_2) = 0.5$. One can quickly check that these are right moving and thus fulfill a WSL. However the SSL can be violated. Let us denote $\Delta p_\nu = p_\nu(t_2) - p_\nu(t_1)$. From (5.11) it follows that

$$\Delta p_1 = J_{12}^{\psi_0}(t) + J_{13}^{\psi_0}(t) = -0.3, \quad (5.14)$$

$$\Delta p_2 = -J_{12}^{\psi_0}(t) + J_{23}^{\psi_0}(t) = -0.1, \quad (5.15)$$

$$\Delta p_3 = -J_{13}^{\psi_0}(t) - J_{23}^{\psi_0}(t) = 0.4. \quad (5.16)$$

This can be true for several choices of $J_{\nu\nu'}^{\psi_0}(t)$, for instance $J_{13}^{\psi_0}(t) = -0.4, J_{12}^{\psi_0}(t) = 0.1$ and $J_{32}^{\psi_0}(t) = 0$. However $J_{13}^{\psi_0}(t) = -0.4$ violates the SSL.

Remark 5.2.2 (Local Detailed Balance). Another conjecture, which discusses similar concepts as we do, was proposed by van Kampen [295] and recently build on by Strassberg et al. [263]. It says that if one considers repeated measurements of $\hat{P}_\nu$ for distinct time steps in an interval $[0, T]$, then the probability distribution of the outcomes is approximated by a Markov process on the macro spaces ν , whose distribution at time t should agree with $\|\hat{P}_\nu \psi_t\|^2$. This conjecture supports the claim, that right moving should be expected, since it suggests that the $\|\hat{P}_\nu \psi_t\|^2$ move approximately like the distribution of a Markov process on the set $\mathcal{N}$ of macrostates,

$$\frac{dp_\nu}{dt} = \sum_{\nu'} (\sigma_{\nu\nu'} p_{\nu'}(t) - \sigma_{\nu'\nu} p_\nu(t)) \quad (5.17)$$

with jump rates $\sigma_{\nu\nu'}$ given for $\nu \neq \nu'$ by

$$\sigma_{\nu\nu'} = \frac{1}{\tau d_{\nu'}} \text{tr}(e^{i\hat{H}\tau} \hat{P}_\nu e^{-i\hat{H}\tau} \hat{P}_{\nu'}) \quad (5.18)$$

for $\tau > 0$ small (such that expression does not depend much on τ), but not too small (or else $\sigma_{\nu\nu'} = 0$). Note that by comparing with (5.8) one sees that

$$J_{\nu\nu'}(t) = \sigma_{\nu\nu'} p_{\nu'}(t) - \sigma_{\nu'\nu} p_\nu(t). \quad (5.19)$$

The so called hypothesis of local detailed balance reads

$$\frac{\sigma_{\nu\nu'}}{\sigma_{\nu'\nu}} \approx \frac{d_\nu}{d_{\nu'}}. \quad (5.20)$$

Whether these last three statements (5.17)-(5.20) are valid in general remains to be open. For certain Wigner matrix models this is the case (see Section 6.2). $\diamond$

5.3. Approximate Entropy Increase

Following the conjecture 4.1 above, we stated versions of the second law, which allow for small violations of entropy increase, as long as these are infrequent, shallow and short lived. The approach we take, by trying to quantify these violations, is not too technical, but not too vague either. It will allow us to capture the necessary aspects, such that we can speak of an **approximate** increase of (4.13). In Section 6.2, we illustrate this idea for a particular random matrix model.

Let us start with some examples and then explain the basic principle. The WSL and SSL hold only approximately. Both make use of the fact that more probability is transported to macro spaces with higher dimension than to lower dimension. This can be expressed as follows. Let

$$\delta_\ell(t) := \int_0^t dt' \sum_\nu \sum_{\nu < \nu'} [J_{\nu\nu'}^{\psi_0}(t')]^+ \quad (5.21)$$

denote the probability flowing to the left (indicated by the ℓ) of ν' , i.e., to smaller subspaces and

$$\delta_r(t) := \int_0^t dt' \sum_\nu \sum_{\nu > \nu'} [J_{\nu\nu'}^{\psi_0}(t')]^+ \quad (5.22)$$

denote the probability flowing to larger subspaces, that is to the right (indicated by the r) of ν' ; here $x^+ = \max(0, x)$ denotes the positive part. In both cases the double sum is understood as summing over the pairs (ν, ν') such that $\nu' < \nu$ and $\nu' > \nu$

respectively. Now the SSL holds approximately if $\delta_\ell(t) \ll \delta_r(t)$, which means that

$$\delta_p(t) = \frac{\delta_\ell(t)}{\delta_r(t)} \ll 1 \quad (5.23)$$

for suitable $t \in [0, T]$.

Another example using the expected decrease/increase of entropy. Let

$$\delta_\ell^S(t') = \int_0^{t'} dt \sum_\nu \sum_{\nu < \nu'} |S_{\nu'} - S_\nu| [J_{\nu\nu'}^{\psi_0}(t)]^+. \quad (5.24)$$

denote the expected decrease of entropy and let

$$\delta_r^S(t') := \int_0^{t'} dt \sum_\nu \sum_{\nu > \nu'} |S_{\nu'} - S_\nu| [J_{\nu\nu'}^{\psi_0}(t)]^+. \quad (5.25)$$

denote the the expected entropy increase. Now we say that the second law holds approximately if $\delta_\ell^S(t) \ll \delta_r^S(t)$, that is we define a quantity

$$\delta^S(t) := \frac{\delta_\ell^S(t)}{\delta_r^S(t)}, \quad (5.26)$$

such that $\delta^S(t) \ll 1$ for suitable $t \in [0, T]$.

Inspired by these examples we now state the general approach: given a reasonable choice of $\hat{H}$, decomposition $\mathcal{H}_{\text{mc}} = \bigoplus_\nu \mathcal{H}_\nu$, initial macro state ν_0 , and $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$, one can define a quantity $\delta(t)$ for $t \in [0, T]$, where T is the time scale of reaching MATE, that captures the violations of entropy increase. We say that the second law approximately holds, if $\delta(t) \ll 1$ for $t \in [0, T]$. Also note that it only says something about the violations until MATE is reached and will not capture fluctuations out of equilibrium afterwards.

Now let us look at a concrete example: Wigner matrices.

6. Second Law for Wigner Matrix Models

In this chapter we consider Wigner matrix models as a reasonable choice for $\hat{H}$ and show that they satisfy a WSL and SSL. In Section 6.1 we check the conditions for a distribution to be right moving in a more general setting applicable to all the cases we discuss afterwards. Now, in Section 6.2, we formulate the WSL and SSL for Wigner matrices. In Section 6.3 we derive a WSL for Wigner type matrices.

6.1. RMD Condition

Let us begin with a condition that appears again and again in this chapter. Here typical weights will be computed for different reasonable setups. They show a key similarity, which we now discuss. In this section let $\mathcal{H}$ be a D -dimensional Hilbert space, $\mathcal{H} = \bigoplus_{\nu} \mathcal{H}_{\nu}$ and let $[K]$ denote the set $\{1, \dots, K\}$.

As we will see for the cases below, under given conditions, the typical evolution of the weights is given by

$$\|\hat{P}_{\nu}\psi_t\|^2 = \frac{d_{\nu}}{D} + f(t) \left(\delta_{\nu\nu_0} - \frac{d_{\nu}}{D} \right). \quad (6.1)$$

In order to fulfill the WSL 5.1, we need to check whether (5.4) is satisfied for (6.1). For $t_2 \geq t_1$ with $t_1, t_2 \in [0, T]$ this leads to

$$\sum_{\nu \geq \nu'} (f(t_2) - f(t_1)) \left(\delta_{\nu\nu_0} - \frac{d_{\nu}}{D} \right) \geq 0. \quad (6.2)$$

Thus whether (6.2) holds one has to distinguish two cases, which depend on the monotonic properties of $f(t)$. In the following let I, I' denote two time intervals, which not necessarily have to be equal to $[0, T]$.

At first consider $t_2 \geq t_1$ and $t_1, t_2 \in I$, such that $f(t_2) - f(t_1) \geq 0$. Thus for (6.2) to hold we need

$$\sum_{\nu \geq \nu'} \left(\delta_{\nu\nu_0} - \frac{d_{\nu}}{D} \right) \geq 0. \quad (6.3)$$

This is true for $\nu_0 \geq \nu'$, as in this case

$$D \geq \sum_{\nu \geq \nu'} d_\nu. \quad (6.4)$$

In that case the probability at time t_2 to be to the right of ν' is larger than the probability at time t_1 . This means that the columns of the histogram to right of ν_0 decrease. It is violated for $\nu_0 < \nu'$, as

$$-\sum_{\nu \geq \nu'} \frac{d_\nu}{D} \geq 0 \quad (6.5)$$

is trivially wrong.

Second, consider $t_2 \geq t_1$ and $t_1, t_2 \in I'$, such that $f(t_2) - f(t_1) \leq 0$. Thus for (6.2) to hold we need

$$\sum_{\nu \geq \nu'} \left(\delta_{\nu\nu_0} - \frac{d_\nu}{D} \right) \leq 0. \quad (6.6)$$

This is true for $\nu_0 < \nu'$ as in this case

$$-\sum_{\nu \geq \nu'} \frac{d_\nu}{D} \leq 0, \quad (6.7)$$

meaning that columns of the histograms to the right of ν_0 are increasing.

It does not hold for $\nu_0 \geq \nu'$, since

$$D \leq \sum_{\nu \geq \nu_0} d_\nu, \quad (6.8)$$

cannot be true as D is the total dimension. This means that histograms to the right of ν' do not increase.

6.2. Second Law for Wigner Hamiltonians

We begin by stating the WSL for Wigner Hamiltonians. These are defined as follows. We take the decomposition and the initial micro state and macro state as fixed and assume $\hat{H}$ to be a Wigner matrix [95]. A **Wigner matrix** $\hat{H} = (h_{ij})$ with $i, j \in [D]$ is a complex $D \times D$ hermitian random matrix with (apart from the hermitian symmetry) independent and identically distributed entries, where

$$\mathbb{E}h_{ij} = 0 \quad \text{and} \quad \mathbb{E}|h_{ij}|^2 = \frac{1}{D}. \quad (6.9)$$

In particular let $\mathbb{P}_{\text{Wig}}$ denote the probability measure on the entries of $\hat{H}$ with the just stated characteristics (see [95] for more details). Note that there are more specific varieties of Wigner matrices, which have a other characteristics as the ones just stated (for more details see [91]). It is well known [91, 95] that for large D the density of the typical empirical distribution of the eigenvalues of a Wigner matrix $\hat{H}$ is given by the Wigner semicircle density

$$\rho_{\text{sc}}(x) = \frac{1}{2\pi} \sqrt{4 - x^2}. \quad (6.10)$$

We will now state the WSL for Wigner matrices and derive it afterwards.

WSL for Wigner matrices: Let $\varepsilon > 0$. Let $\mathcal{H}_{\text{mc}} = \bigoplus_{\nu} \mathcal{H}_{\nu}$ be a decomposition of the energy shell, let ν, ν_0 be two arbitrary macro states and let $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$. Further let $\hat{H}$ be a Wigner matrix. Then for $T > 0$ and D large enough, $(1 - \varepsilon)$ -most $\hat{H}$ are such that

$$\|\hat{P}_{\nu}\psi_t\|^2 = \frac{d_{\nu}}{D} + \left(\frac{J_1(2t)}{t}\right)^2 \left(\delta_{\nu\nu_0} - \frac{d_{\nu}}{D}\right), \quad (6.11)$$

which is a family $(p_{\nu}(t))_{t \in [0, T]}$ of ARMDs up to time T .

We now derive the WSL. Using a result from Cipolloni et al. [65], we compute the weights for a Wigner Hamiltonian. Afterwards we argue that these weights yield a family of ARMDs.

In [65] Cipolloni et al. showed that modelling the Hamiltonian as a Wigner matrix yields crucial estimates concerning thermalization with respect to certain observables. Here we make use of the following result: for a bounded deterministic observable $\hat{A}$, evolving in time as $\hat{A}(t) = e^{i\hat{H}t}\hat{A}(0)e^{-i\hat{H}t}$, fixed deterministic vectors $\psi, \phi \in \mathbb{C}^D$, and $\xi > 0$,

$$\langle \psi | \hat{A}(t) | \phi \rangle = \langle \psi | \phi \rangle \frac{\text{tr } \hat{A}}{D} + \frac{\theta^2(t)}{t^3} \langle \psi | \left(\hat{A} - \frac{\text{tr } \hat{A}}{D} \right) | \phi \rangle + \mathcal{O}(D^{\xi-1/2}t^2), \quad (6.12)$$

holds with very high probability (w.v.h.p.). Further $\theta(t) := J_1(2t)\sqrt{t}$, where $J_1(x)$ is the Bessel function of first kind.

Applying this to our setting, that is $\hat{A} = \hat{P}_{\nu}$, $\hat{A}(t) = e^{i\hat{H}t}\hat{P}_{\nu}e^{-i\hat{H}t}$, $\psi = \phi = \psi_0$ and thus $\langle \psi | \hat{A}(t) | \phi \rangle = \|\hat{P}_{\nu}\psi_t\|^2$. Further $\text{tr } \hat{P}_{\nu} = d_{\nu}$. After a quick calculation, noting that for $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$ we get $\langle \psi_0 | \hat{P}_{\nu} | \psi_0 \rangle = \delta_{\nu\nu_0}$, one immediately obtains with $\xi > 0$,

$$\|\hat{P}_{\nu}\psi_t\|^2 = \frac{d_{\nu}}{D} + \left(\frac{J_1(2t)}{t}\right)^2 \left(\delta_{\nu\nu_0} - \frac{d_{\nu}}{D}\right) + \mathcal{O}(D^{\xi-1/2}t^2), \quad (6.13)$$

which again holds w.v.h.p. This is understood as follows. The goal is to find a typicality statement about $\hat{H}$ of the following form. Let $\text{HM}(\mathcal{H})$ denote the set of hermitian matrices on $\mathcal{H}$ and let $\mathbb{P}_{\text{Wig}}$ denote the measure on the entries of $\hat{H}$. For $\varepsilon > 0$ a statement $s(\hat{H})$ is true for $(1 - \varepsilon)$ -most $\hat{H}$ if and only if

$$\mathbb{P}_{\text{Wig}}\left(\{\hat{H} \in \text{HM}(\mathcal{H}) : s(\hat{H}) \text{ holds}\}\right) \geq 1 - \varepsilon \quad (6.14)$$

To get such a statement we first define

$$w_\nu(t) = \frac{d_\nu}{D} + \left(\frac{J_1(2t)}{t}\right)^2 \left(\delta_{\nu\nu_0} - \frac{d_\nu}{D}\right) \quad (6.15)$$

and thus w.v.h.p.

$$\|\hat{P}_\nu \psi_t\|^2 - w_\nu(t) = \mathcal{O}(D^{\xi-1/2}t^2). \quad (6.16)$$

This means that there exists $\gamma > 0$ and $C = C(\xi, D) > 0$, such that

$$\mathbb{P}_{\text{Wig}}\left(\|\|\hat{P}_\nu \psi_t\|^2 - w_\nu(t)\| < CD^{\xi-1/2}t^2\right) \geq 1 - D^{-\gamma}. \quad (6.17)$$

Now this means that for $(1 - \varepsilon)$ -most $\hat{H}$ with $D > D_0(\varepsilon, \gamma) = \varepsilon^{-1/\gamma}$

$$\|\|\hat{P}_\nu \psi_t\|^2 - w_\nu(t)\| < CD^\xi \frac{t^2}{\sqrt{D}}. \quad (6.18)$$

As $D \propto e^N$, where N is the particle number (this follows from the extensivity of entropy) it follows that the random fluctuation is small given that

$$t \ll D^{\frac{1}{4} - \frac{\varepsilon}{2}} \propto e^{N(1-2\varepsilon)/4}, \quad (6.19)$$

which is the case for suitable ε and N large enough. From here on we simply consider such times and thus need to check next whether (6.15) yields a family of ARMDs, that is whether it fullfills (5.4). In the following we use the abbreviation

$$\varphi_1(t) := \frac{J_1(2t)}{t}. \quad (6.20)$$

Let $t_2 \geq t_1$ with $t_1, t_2 \in [0, T]$ and ν' some fixed macro state, and thus (5.4) reads

$$(\varphi_1^2(t_2) - \varphi_1^2(t_1)) \sum_{\nu \geq \nu'} \left(\delta_{\nu\nu_0} - \frac{d_\nu}{D}\right) \geq 0. \quad (6.21)$$

Hence it boils down to the monotonic properties of $\varphi_1^2(t)$. This needs a more detailed discussion, since $\varphi_1^2(t)$ is neither monotonically decreasing, nor monotonically

increasing, but essentially its decreasing, as can be seen from Figure 6.1. We refer to the first section of this chapter.

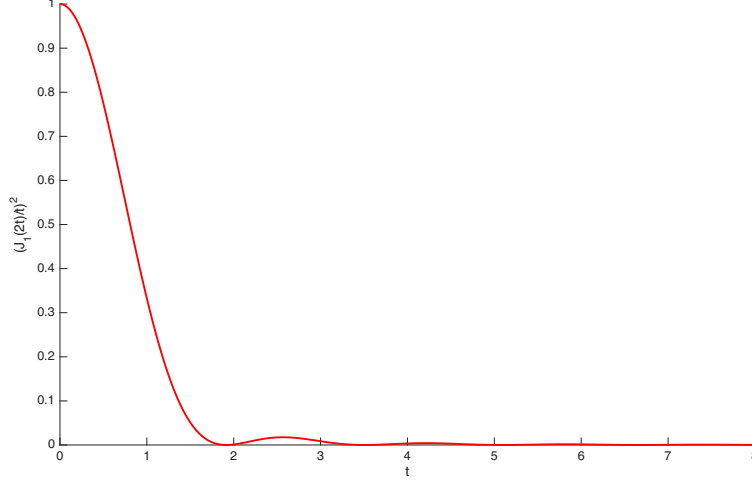


Figure 6.1.: The function $\varphi_1^2(t)$ with its quickly decaying behavior. The function shows oscillatory behaviour, but the amplitudes are so small compared to the maximum value $\varphi_1^2(0) = 1$, such that the function is "approximately" decreasing.

Before that we use the fact that for large enough times one can rewrite (6.20) as [65, Eq.1.5]

$$\varphi_1^2(t) = \frac{\theta^2(t)}{t^3} \quad \text{with} \quad \theta(t) = J_1(2t)\sqrt{t}. \quad (6.22)$$

The reason to do this is that $\theta(t)$ is an oscillatory function of order one, which means that the essential time behavior of (6.22) is given by t^{-3} . This is due to a basic property of Bessel functions [65, Eq.2.7]: for $x \gg 1$,

$$J_1(x) = -\cos\left(x + \frac{\pi}{4}\right) \sqrt{\frac{2}{\pi x}} + \mathcal{O}(x^{-3/2}). \quad (6.23)$$

Without these oscillations, one would immediately see that (6.21) for $t_2 \geq t_1$ with t_1, t_2 sufficiently large and ν' some fixed macro state reads

$$\left(\frac{1}{t_2^3} - \frac{1}{t_1^3}\right) \sum_{\nu \geq \nu'} \left(\delta_{\nu\nu_0} - \frac{d_\nu}{D}\right) \geq 0 \quad (6.24)$$

and thus holds given that

$$\sum_{\nu \geq \nu'} \left(\delta_{\nu\nu_0} - \frac{d_\nu}{D}\right) \leq 0, \quad (6.25)$$

which is true for $\nu_0 < \nu'$, but for $\nu' \leq \nu_0$ the condition is violated.

Let's get back to the more general case and take not only large times into account. We now apply the reasoning from Section 6.1. We denoted the zeroes and the local maxima of $\varphi_1^2(t)$ in Figure 6.2. That is for instance let $t \in [T_0, T_1)$, then the function $\varphi_1^2(t)$ is decreasing and thus the RMD condition holds for $\nu_0 < \nu'$ and is violated for $\nu' \geq \nu_0$. This means that the columns of the histograms to the right of ν_0 rise.

For $t \in [T_1, T_2)$ the function $\varphi_1^2(t)$ is increasing and thus the RMD condition holds for $\nu_0 \geq \nu'$ and is violated for $\nu_0 < \nu'$. That means probability is transported to the left of ν_0 and therefore violates the second law. Similar arguments can be made for further time intervals applying the reasoning from Section 6.1.

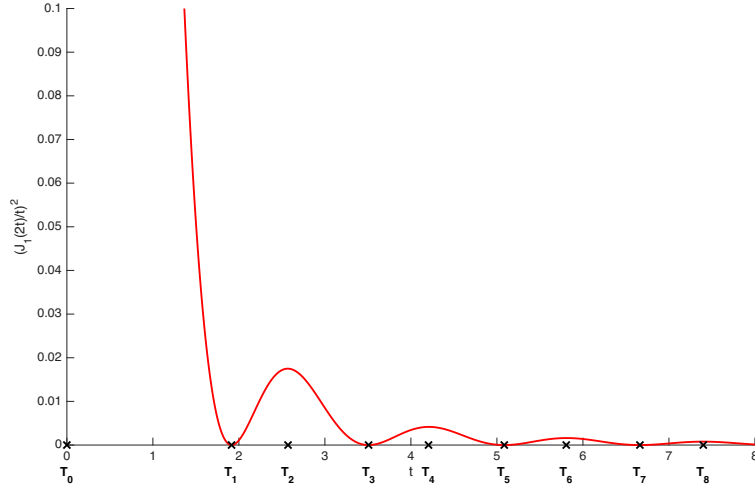


Figure 6.2.: The local maxima of $\varphi_1^2(t)$ are denoted by $T_{2i} = j_{2,i}/2$ with $i \in \{0, 1, 2, 3, 4\}$ and $j_{2,n}$ the zeroes of the Bessel function $J_2(x)$. The local minima (zeroes) of $\varphi_1^2(t)$ are denoted by $T_{2i+1} = j_{1,i}/2$ where $j_{1,n}$ are the zeroes of the Bessel function $J_1(x)$ with $i \in \{0, 1, 2, 3\}$. The height of the local maxima of $\varphi_1^2(t)$ decrease as t increases and already the first local maxima is much smaller, than the global maximum $\varphi_1^2(0) = 1$.

In order to check that these weights are approximately right moving we use the current $J_{\nu\nu'}^{\psi_0}(t)$, which we compute using results from Cipolloni et al. [64]. The considerations are similar as for the weights (we explain the reason below in section 7.1).

In order to compute the current, recall that it is given by

$$J_{\nu\nu'}^{\psi_0}(t) = -i\langle\psi_0|e^{i\hat{H}t}\hat{P}_\nu\hat{H}\hat{P}_{\nu'}e^{-i\hat{H}t}|\psi_0\rangle \quad (6.26)$$

$$+ i\langle\psi_0|e^{i\hat{H}t}\hat{P}_{\nu'}\hat{H}\hat{P}_\nu e^{-i\hat{H}t}|\psi_0\rangle. \quad (6.27)$$

Here we apply another result of Cipolloni et al. [64, Ex. 2.8] to obtain a deterministic

approximation of $J_{\nu\nu'}^{\psi_0}(t)$. In the notation used there, we consider the case $k = 3$, where $W = \hat{H}$, $A_i = \hat{P}_\nu$, $f_1(x) = e^{ixt}$, $f_2(x) = x$ and $f_3(x) = e^{-ixt}$. Treating the two summands in (6.26) separately we first note that w.v.h.p.

$$-i\langle\psi_0|e^{i\hat{H}t}\hat{P}_\nu\hat{H}\hat{P}_{\nu'}e^{-i\hat{H}t}|\psi_0\rangle = -i\langle\psi_0|F_3(\nu, \nu')|\psi_0\rangle \quad (6.28)$$

$$+ \mathcal{O}(D, t) \quad (6.29)$$

$$i\langle\psi_0|e^{i\hat{H}t}\hat{P}_{\nu'}\hat{H}\hat{P}_\nu e^{-i\hat{H}t}|\psi_0\rangle = i\langle\psi_0|F_3(\nu', \nu)|\psi_0\rangle \quad (6.30)$$

$$+ \mathcal{O}(D, t), \quad (6.31)$$

where $F_3(\nu, \nu')$ and $F_3(\nu', \nu)$ are the respective deterministic approximations of the random quantities in (6.26) and $\mathcal{O}(D, t) = \mathcal{O}(g(D, t))$, where $g(D, t)$ is a function not important here, we will define it below. As $F_3(\nu', \nu)$ appears from $F_3(\nu, \nu')$ simply by interchanging ν and ν' , we focus only on $F_3(\nu, \nu')$, which reads

$$F_3(\nu, \nu') = \hat{P}_\nu \hat{P}_{\nu'} \text{sc}_o[1] \text{sc}_o[2] \text{sc}_o[3] \quad (6.32)$$

$$+ \text{tr}(\hat{P}_\nu \hat{P}_{\nu'}) \text{sc}_o[1, 3] \text{sc}_o[2] \quad (6.33)$$

$$+ \hat{P}_\nu \text{tr}(\hat{P}_{\nu'}) \text{sc}_o[1] \text{sc}_o[2, 3] \quad (6.34)$$

$$+ \hat{P}_{\nu'} \text{tr}(\hat{P}_\nu) \text{sc}_o[1, 2] \text{sc}_o[3] \quad (6.35)$$

$$+ \text{tr}(\hat{P}_\nu) \text{tr}(\hat{P}_{\nu'}) \text{sc}_o[1, 2, 3], \quad (6.36)$$

with

$$\text{sc}_o[i] = \langle f_i \rangle_{\text{sc}} \quad (6.37)$$

$$\text{sc}_o[i, j] = \langle f_i f_j \rangle_{\text{sc}} - \langle f_i \rangle_{\text{sc}} \langle f_j \rangle_{\text{sc}} \quad (6.38)$$

$$\text{sc}_o[1, 2, 3] = \langle f_1 f_2 f_3 \rangle_{\text{sc}} - \langle f_1 f_2 \rangle_{\text{sc}} \langle f_3 \rangle_{\text{sc}} \quad (6.39)$$

$$- \langle f_1 f_3 \rangle_{\text{sc}} \langle f_2 \rangle_{\text{sc}} - \langle f_2 f_3 \rangle_{\text{sc}} \langle f_1 \rangle_{\text{sc}} \quad (6.40)$$

$$+ 2\langle f_1 \rangle_{\text{sc}} \langle f_2 \rangle_{\text{sc}} \langle f_3 \rangle_{\text{sc}} \quad (6.41)$$

where

$$\langle f \rangle_{\text{sc}} = \int_{-2}^2 dx f(x) \rho_{\text{sc}}(x) \quad (6.42)$$

and $\rho_{\text{sc}}(x) = (1/2\pi)\sqrt{4-x^2}$ the semicircle density.

After an elementary calculation of (6.37-6.39) one finds with

$$\langle f_1 \rangle_{\text{sc}} = \langle f_3 \rangle_{\text{sc}} = \frac{J_1(2t)}{t} \quad (6.43)$$

$$\langle f_2 \rangle_{\text{sc}} = \langle f_1 f_2 f_3 \rangle_{\text{sc}} = 0 \quad (6.44)$$

$$\langle f_1 f_3 \rangle_{\text{sc}} = 1 \quad (6.45)$$

$$\langle f_2 f_3 \rangle_{\text{sc}} = -\langle f_1 f_2 \rangle_{\text{sc}} = -\frac{i}{2} \frac{J_2(2t)}{t} \quad (6.46)$$

and $\text{tr}(\hat{P}_\nu \hat{P}_{\nu'})/D = d_\nu \delta_{\nu\nu'}/D$, such that

$$F_3(\nu, \nu') = \frac{2i}{D} \frac{J_1(2t)J_2(2t)}{t^2} (\hat{P}_{\nu'} d_\nu - \hat{P}_\nu d_{\nu'}). \quad (6.47)$$

Further for $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$, note that $\langle \psi_0 | \hat{P}_{\nu'} | \psi_0 \rangle = \delta_{\nu'\nu_0}$ and thus

$$\langle \psi_0 | F_3(\nu, \nu') | \psi_0 \rangle = \frac{2i}{D} \frac{J_1(2t)J_2(2t)}{t^2} (\delta_{\nu'\nu_0} d_\nu - \delta_{\nu\nu_0} d_{\nu'}). \quad (6.48)$$

By flipping ν and ν' one obtains the respective expression for $F_3(\nu', \nu)$ and one finds that

$$J_{\nu\nu'}^{\psi_0}(t) = -i\langle \psi_0 | F_3(\nu, \nu') | \psi_0 \rangle + i\langle \psi_0 | F_3(\nu', \nu) | \psi_0 \rangle + \mathcal{O}(D, t) \quad (6.49)$$

$$= \frac{4}{D} (d_\nu \delta_{\nu_0\nu'} - d_{\nu'} \delta_{\nu\nu_0}) \frac{J_1(2t)J_2(2t)}{t^2} + \mathcal{O}(D, t), \quad (6.50)$$

holds w.v.h.p. As for the weights above we are interested in statements, which say that most $\hat{H}$ are such that the current is with high probability given by the expression above. Let's do that. Now here $\mathcal{O}(D, t)$ is, as above, a random quantity, which for any $\xi > 0$ by [65, Cor. 2.9] reads

$$\mathcal{O}(D, t) = \mathcal{O}(D^{\xi-1/2} t^3). \quad (6.51)$$

This means there exists a $\gamma' > 0$ and $K = K(\xi, \gamma') > 0$, such

$$\mathbb{P}_{\text{Wig}} \left\{ |J_{\nu\nu'}^{\psi_0}(t) - C_{\nu\nu'}^{\psi_0}(t)| < K D^{\xi-1/2} t^3 \right\} \geq 1 - D^{-\gamma'}, \quad (6.52)$$

where

$$C_{\nu\nu'}^{\psi_0}(t) = \frac{4}{D} (d_\nu \delta_{\nu_0\nu'} - d_{\nu'} \delta_{\nu\nu_0}) \frac{J_1(2t)J_2(2t)}{t^2}. \quad (6.53)$$

This allows us to say that $(1 - \varepsilon')$ -most $\hat{H}$ with $D > D_0(\varepsilon', \gamma) = (\varepsilon')^{-1/\gamma'}$ are such that

$$|J_{\nu\nu'}^{\psi_0}(t) - C_{\nu\nu'}^{\psi_0}(t)| < K D^{\xi-1/2} t^3. \quad (6.54)$$

Thus as $t \ll D^{(1/6-\xi/3)}$ for D large enough (here again $D \propto e^N$, with N the number of particles) we obtain the final result

$$J_{\nu\nu'}^{\psi_0}(t) = \frac{4}{D} (d_\nu \delta_{\nu_0\nu'} - d_{\nu'} \delta_{\nu\nu_0}) \varphi_1(t) \varphi_2(t), \quad (6.55)$$

where we used (6.20) and defined

$$\varphi_2(t) := \frac{J_2(2t)}{t}. \quad (6.56)$$

As $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$, this means that probability is flowing away from ν_0 to every ν at a rate proportional to d_ν/D . Entropy increases if more probability is flowing from smaller ν to larger ν' . We first use the current to finalize the WSL.

We now show that the current is overwhelmingly pointing to larger subspaces. To this end we use (5.21) and (5.22), which using (6.55), reads

$$\delta_\ell(t) = \frac{4}{D} \left[\int_0^t dt' \sum_{\nu < \nu_0} d_\nu (\varphi_1(t') \varphi_2(t'))^+ + \sum_{\nu_0 < \nu'} d_{\nu'} (\varphi_1(t') \varphi_2(t'))^- \right], \quad (6.57)$$

$$\delta_r(t) = \frac{4}{D} \left[\int_0^t dt' \sum_{\nu > \nu_0} d_\nu (\varphi_1(t') \varphi_2(t'))^+ + \sum_{\nu_0 > \nu'} d_{\nu'} (\varphi_1(t') \varphi_2(t'))^- \right], \quad (6.58)$$

where $x^- = \min(0, x)$ and $x^+ = \max(0, x)$. We need that $\delta_\ell(T) \ll \delta_r(T)$, hence

$$\delta(T) = \frac{\delta_\ell(T)}{\delta_r(T)} \ll 1. \quad (6.59)$$

To show this, we first define

$$\xi^-(T) := \int_0^T dt (\varphi_1(t) \varphi_2(t))^- , \quad (6.60)$$

$$\xi^+(T) := \int_0^T dt (\varphi_1(t) \varphi_2(t))^+ , \quad (6.61)$$

$$\kappa(T) := \frac{\xi^-(T)}{\xi^+(T)}. \quad (6.62)$$

Now note that due to the large dimensions, we have

$$\sum_{\nu' < \nu_0} d_{\nu'} \ll \sum_{\nu_0 < \nu'} d_{\nu'} \quad (6.63)$$

and thus

$$\delta(T) \approx \kappa(T) \ll 1 \quad (6.64)$$

for sufficiently large T . More precisely (using standard computer programmes, for

example Wolframalpha), one finds that⁴⁴

$$\lim_{T \rightarrow \infty} \xi^+(T) \approx 0.25638, \quad (6.65)$$

$$\lim_{T \rightarrow \infty} \xi^-(T) \approx 0.00639 \quad (6.66)$$

and therefore

$$\lim_{T \rightarrow \infty} \kappa(T) \approx \mathcal{O}(10^{-2}). \quad (6.67)$$

That is violations are of the order of a percent. Therefore the WSL holds and also the SSL.

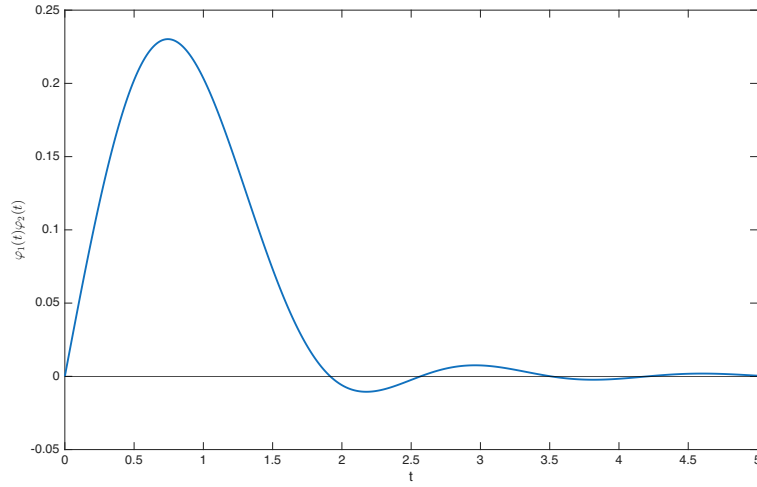


Figure 6.3.: The plot shows the function $\varphi_1(t)\varphi_2(t)$.

Finally, the Wigner SSL reads

SSL for Wigner matrices: Let $\varepsilon' > 0$. For $\mathcal{H}_{\text{mc}} = \bigoplus_{\nu} \mathcal{H}_{\nu}$, arbitrary $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$ and ν_0 , for $(1 - \varepsilon')$ -most $\hat{H}$ and sufficiently large D the current (6.55) points overwhelmingly from smaller $\mathcal{H}_{\nu}$ to larger $\mathcal{H}_{\nu'}$.

To fulfill the SSL 5.2 we need to show that $J_{\nu\nu'}^{\psi_0}(t) \leq 0$. This is roughly the case for $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu})$, so $\nu_0 \neq \nu'$ and $\nu_0 = \nu$, then the current reads

$$J_{\nu_0\nu'}^{\psi_0}(t) = -4 \frac{d_{\nu'}}{D} \varphi_1(t)\varphi_2(t) \leq 0 \quad (6.68)$$

for $t \in \mathcal{G}$, where $\mathcal{G}$ is the set of times where $\varphi_1(t)\varphi_2(t)$ is positive. Looking at Figure 6.3 makes it clear that (6.68) is indeed positive for a good amount of times.

⁴⁴Since the factor 4 cancels out in $\delta(T)$ one does not obtain a value close to 1, but close to 1/4.

Remark 6.2.1 (Local Detailed Balance for Wigner Matrices). Let ν, ν' be two macro states and let $\hat{H}$ be a Wigner matrix. We apply results from [64] to compute $\sigma_{\nu\nu'}$ and $\sigma_{\nu'\nu}$:

$$\sigma_{\nu\nu'} = \frac{1}{\tau d_{\nu'}} \text{tr}(e^{i\hat{H}\tau} \hat{P}_\nu e^{-i\hat{H}\tau} \hat{P}_{\nu'}) \quad (6.69)$$

$$= \frac{1}{\tau d_{\nu'}} \left(\delta_{\nu\nu'} d_\nu \frac{J_1^2(2\tau)}{\tau^2} + \frac{d_\nu d_{\nu'}}{D} - \frac{d_\nu d_{\nu'}}{D} \frac{J_1^2(2\tau)}{\tau^2} \right), \quad (6.70)$$

$$\sigma_{\nu'\nu} = \frac{1}{\tau d_\nu} \text{tr}(e^{i\hat{H}\tau} \hat{P}_{\nu'} e^{-i\hat{H}\tau} \hat{P}_\nu) \quad (6.71)$$

$$= \frac{1}{\tau d_\nu} \left(\delta_{\nu\nu'} d_{\nu'} \frac{J_1^2(2\tau)}{\tau^2} + \frac{d_\nu d_{\nu'}}{D} - \frac{d_\nu d_{\nu'}}{D} \frac{J_1^2(2\tau)}{\tau^2} \right). \quad (6.72)$$

Hence the fraction $\sigma_{\nu\nu'}/\sigma_{\nu'\nu}$ is given by

$$\frac{\sigma_{\nu\nu'}}{\sigma_{\nu'\nu}} = \frac{\frac{d_\nu}{D} + \frac{J_1^2(2\tau)}{\tau^2} (\delta_{\nu\nu'} - \frac{d_\nu}{D})}{\frac{d_{\nu'}}{D} + \frac{J_1^2(2\tau)}{\tau^2} (\delta_{\nu\nu'} - \frac{d_{\nu'}}{D})}. \quad (6.73)$$

Since $J_1^2(2t)/t^2$ vanishes quickly for $t > 0$ we obtain local detailed balance

$$\frac{\sigma_{\nu\nu'}}{\sigma_{\nu'\nu}} \approx \frac{d_\nu}{d_{\nu'}} \quad (6.74)$$

for sufficiently large τ . $\diamond$

Note that similar results can be obtained from Reimann [222] and Dabelow and Reimann [72]. These concern the weights, but not the current. The results are also typicality statements.

Reimann [222] considered the following setup. Let $\mathcal{H}$ be a Hilbert space, $\hat{H}$ a Hamiltonian and $\hat{\rho}$ a density matrix on $\mathcal{H}$ ($\hat{\rho}$ can either be pure or mixed). As usual the relevant part of $\mathcal{H}$ is given by the energy shell $\mathcal{H}_{\text{mc}}$. The space spanned by those eigenvectors with eigenvalues in $[E - \Delta E, E]$; where $\Delta E > 0$ small on the macroscopic scale, but large enough to contain many eigenvalues, such that $\dim \mathcal{H}_{\text{mc}} = D$ is still finite, but large. Let further $\hat{A}$ be a self-adjoint operator on $\mathcal{H}_{\text{mc}}$ with expectation value

$$\text{tr}(\hat{\rho}(t)\hat{A}) = \sum_{n,m} \hat{\rho}_{mn}(0) \hat{A}_{nm} e^{it(E_n - E_m)}, \quad (6.75)$$

where $\hat{\rho}_{mn}(t) = \langle \phi_n | \hat{\rho}(t) | \phi_m \rangle$ and $\hat{A}_{nm} = \langle \phi_m | \hat{A} | \phi_n \rangle$.

Let $\hat{U} : \mathcal{H}_{\text{mc}} \rightarrow \mathcal{H}_{\text{mc}}$ be a unitary matrix, which relates the eigenbasis of $\hat{A}$ and $\hat{H}$, while considering the basis of $\hat{\rho}(0)$ to $\hat{A}$ as fixed. Now assume that $\hat{U}$ is distributed according to the Haar measure (see Section 2.3). The main result of [222] is that for

most $\hat{U}$ and most times $t \in [0, T]$

$$\text{tr}(\hat{\rho}(t)\hat{A}) = \text{tr}(\hat{\rho}_{\text{mc}}\hat{A}) + F(t)\{\text{tr}(\hat{\rho}(0)\hat{A}) - \text{tr}(\hat{\rho}_{\text{mc}}\hat{A})\}, \quad (6.76)$$

where

$$F(t) = |\Phi(t)|^2 \quad \text{with} \quad \Phi(t) = \frac{1}{D} \sum_{n=1}^D e^{iE_n t}. \quad (6.77)$$

As an example Reimann considered the density $\rho(E - y) = ce^{-y\beta}$ to derive for $\Delta E \gg k_B T$ that

$$F(t) = \frac{1}{1 + (k_B T t)^2}. \quad (6.78)$$

This can be applied to our setting in the following way: $\hat{A} = \hat{P}_\nu$, $\hat{\rho}(t) = |\psi_t\rangle\langle\psi_t|$, $\text{tr}(\hat{P}_\nu\hat{\rho}(t)) = \|\hat{P}_\nu\psi_t\|^2$ and $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$. Then for most $\hat{U}$ and most times $t \in [0, T]$

$$\|\hat{P}_\nu\psi_t\|^2 = \frac{d_\nu}{D} + F(t)\left(\delta_{\nu\nu_0} - \frac{d_\nu}{D}\right). \quad (6.79)$$

It can be easily seen (with the reasoning in Section 6.1) that for $F(t)$ as in (6.78) the weights (6.79) lead to a family of RMDs and thus to a WSL.

In [72], Dabelow and Reimann, consider the typical evolution of (6.75) for a Hamiltonian of the form

$$\hat{H} = \hat{H}_0 + \lambda\hat{V} \quad (6.80)$$

where $\hat{V}$ is a GUE matrix, more specifically

$$\mathbb{E}v_{nm} = 0 \quad \text{and} \quad \mathbb{E}|v_{nm}|^2 = \sigma_V^2 f(|n - m|) \quad (6.81)$$

where $\hat{V}_{nm} = \langle\phi_n|\hat{V}|\phi_m\rangle$ in the basis of the eigenvectors of $\hat{H}_0$, where $\hat{H}_0|\phi_n\rangle = E_n|\phi_n\rangle$. They assume that the mean level spacing of energy levels in $[E - \Delta E, E]$ is constant, and denoted as η , i.e., the density of states is $\rho(E) = 1/\eta$. The function $f(|n - m|)$ describes the band profile of $\hat{V}$ and σ_V is a constant, the bandwidth is given by B (for all the details see [72]). In our case the band profile expresses that different subspaces are coupled at different “ strengths”.

Remark 6.2.2. Interactions play a key role in the approach to thermal equilibrium. Here this can be seen as follows: suppose that $\hat{H}_0$ is block-diagonal, that is $\hat{H}_0$ consists of blocks $\hat{H}_{0,\nu}$, such that for each ν the block $\hat{H}_{0,\nu}$ is diagonal in $\mathcal{H}_\nu$, i.e., $[\hat{H}_0, \hat{P}_\nu] = 0$ for each $\nu \in \mathcal{N}$. This immediately shows that the off-diagonal elements of the full Hamiltonian $\hat{H} = \hat{H}_0 + \lambda\hat{V}$, namely the interaction part $\hat{V}$, is responsible for the transitions between the different subspaces. More explicitly, the temporal change in

the weights $||\hat{P}_\nu \psi_t||^2$ is given by

$$\frac{dp_\nu}{dt} = i\langle \psi_t | [\hat{H}, \hat{P}_\nu] | \psi_t \rangle \quad (6.82)$$

$$= i\lambda \langle \psi_t | [\hat{V}, \hat{P}_\nu] | \psi_t \rangle, \quad (6.83)$$

which clearly depends on $\hat{V}$. $\diamond$

The main result in [72] is that for most perturbations $\hat{V}$ and most $t \in [0, T]$ the evolution of (6.75) is given by

$$\text{tr}(\hat{\rho}(t)\hat{A}) = \text{tr}(\hat{\rho}_{\text{mc}}\hat{A}) + |g(t)|^2 \{ \text{tr}(\hat{\rho}_0(t)\hat{A}) - \text{tr}(\hat{\rho}_{\text{mc}}\hat{A}) \} \quad (6.84)$$

where $\hat{\rho}_0(t)$ evolves according to the unperturbed dynamics. The time dependence enters through $g(t)$ in two different ways. For weak perturbations (essentially small bandwidth) one obtains

$$g(t) = e^{-\gamma t/2} \quad (6.85)$$

with $\gamma = \gamma(\lambda, \sigma_V, \eta)$. While for strong perturbations (essentially large band width and “full GUE”)

$$g(t) = 2 \frac{J_1(\alpha t)}{(\alpha t)} \quad (6.86)$$

with $\alpha = \alpha(B, \lambda, \sigma_V)$. As before, it follows by applying it to our case that for weak perturbations, most $\hat{V}$ and most times $t \in [0, T]$ are such that

$$||\hat{P}_\nu \psi_t||^2 = \frac{d_\nu}{D} + e^{-\gamma t} \left(\delta_{\nu\nu_0} - \frac{d_\nu}{D} \right). \quad (6.87)$$

For strong perturbations, for most V and most times $t \in [0, T]$ the weights read

$$||\hat{P}_\nu \psi_t||^2 = \frac{d_\nu}{D} + 4 \frac{J_1^2(\alpha t)}{(\alpha t)^2} \left(\delta_{\nu\nu_0} - \frac{d_\nu}{D} \right). \quad (6.88)$$

The constants γ and α do not bother us here.

Using similar arguments as before and in Section 6.1 we obtain a WSL.

Remark 6.2.3. Note that the results of Reimann and Dabelow just discussed are very similar to the ones obtained above for the Wigner matrices. This is not an accident. Wigner matrices and GUE matrices are closely related. A GUE matrix is a Wigner matrix with Gaussian distributed entries. That is one can speak of Wigner matrices and GUE matrices in a similar vein. $\diamond$

Ultrafast Thermalization

Let us also comment on thermalization times. From Figure 6.1 it can be seen that the weights approach their thermal equilibrium values “relatively fast”. More precisely for $t \gg 1$, we have

$$||\hat{P}_\nu \psi_t||^2 \approx \frac{d_\nu}{D} \quad (6.89)$$

and in particular $\hat{P}_{\text{eq}} \psi_t \approx d_{\text{eq}}/D \approx 1$. The fast thermalization is not a surprise. We have seen in Section 2.6 that for a uniformly distributed subspace, thermalization time scales at room temperature are expected to be of the order of the Boltzmann time

$$\tau_B = \frac{h}{k_B T}. \quad (6.90)$$

For Wigner matrices the ONB of $\hat{H}$ is also uniformly distributed and thus we expect the same results. As we set $\hbar = 1$ we do not have an explicit time scale in our formulas above. The time dependence of $||\hat{P}_\nu \psi_t||^2$ in (6.15) is given by (6.20). Here t is a dimensionless parameter. That has two reasons: first the energy is expressed as the energy per degree of freedom in the semicircle distribution (which first got us (6.15)) and second, as just mentioned, that $\hbar = 1$. That is t in (6.15) has an implicit time scale, which can be restored by substituting t with $(E/hN)t$. As in Section 2.6 we set $E = Nk_B T$ and get as a time scale the Boltzmann time (6.90). That means our result is in line with the one from Section 2.6.

6.3. Weak Second Law for Wigner Type Hamiltonians

Instead of a Wigner matrix we will now consider a Wigner-Type matrix, which has a more general variance profile $\mathbb{E}|h_{ij}|^2$ and therefore mimics a more realistic physical behavior compared to the Wigner matrix. Using results from [93], where they consider the typical behavior of $||\hat{P}_\nu \psi_t||^2$ for two subspaces and three subspaces, we derive a WSL. It is believed that a SSL can also be stated. The calculations are however quite involved. An analytical extension beyond that seems currently out of reach. However, one is still able to write down general expressions, which we do below.

6.3.1. WSL for two Macrospace

Consider $\mathcal{H}_{\text{mc}} = \mathcal{H}_1 \oplus \mathcal{H}_2$ with dimension $D = d_1 + d_2 = (1 + \lambda)d$, where $\lambda > 0$ is a small parameter. Here one can think of $\mathcal{H}_1$ as the non-equilibrium subspace $\mathcal{H}_{\text{neq}}$ and of $\mathcal{H}_2$ as the thermal equilibrium subspace $\mathcal{H}_{\text{eq}}$. The characteristics of the Wigner Type Hamiltonian $\hat{H} = (h_{ij})$ with $i, j \in [D]$ ⁴⁵ are given by its variance matrix (a

⁴⁵Recall that $[D] = \{1, \dots, D\}$.

block matrix)

$$S = (S_{ij}) = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \quad (6.91)$$

with blocks

$$S_{11} = \frac{1}{D\lambda} E_{d_1 d_1}, \quad S_{12} = S_{21}^* = \frac{\lambda}{D} E_{d_1 d_2}, \quad S_{22} = \frac{1 + \lambda - \lambda^2}{D} E_{d_2 d_2} \quad (6.92)$$

where $E_{d_i d_j}$ is the $d_i \times d_j$ matrix carrying ones in each entry⁴⁶.

The entries of the variance matrix S are chosen such that the rows and columns add up to one. The reason is that in this case there exists a solution to the quadratic vector equation, which is linked to the distribution of the eigenvalues of $\hat{H}$ and further plays a key role to find typical weights $\|\hat{P}_\nu \psi_t\|^2$ (for more details see section 7.1). Physically this model allows transitions between $\mathcal{H}_1$ and $\mathcal{H}_2$ at a different “strength”, than in the Wigner model. As there all transition elements, where equally strong, thermalization appears ultrafast (see above), this is not the case here (for a more general discussion see [93]).

According to [93, Thm.2.5] for $\psi_0 \in \mathbb{S}(\mathcal{H}_1)$ the weights read with very high probability

$$\|\hat{P}_1 \psi_t\|^2 = 1 - \frac{d_2}{D} + \frac{1}{\pi(\lambda t)^3} (1 + o(1)) + \mathcal{O}(C(\lambda, t)/\sqrt{D}), \quad (6.93)$$

$$\|\hat{P}_2 \psi_t\|^2 = \frac{d_2}{D} - \frac{1}{\pi(\lambda t)^3} (1 + o(1)) + \mathcal{O}(C(\lambda, t)/\sqrt{D}). \quad (6.94)$$

Here $C(\lambda, t)$ is a constant depending only on its arguments and $o(1)$ vanishes in the limit $t \rightarrow \infty$, $\lambda \rightarrow 0$ and $t\lambda \rightarrow 0$. Consider the case $t \gg 1/\lambda$. Since $\lambda = d_1/d_2$, this means that $t \gg 1$. Further choose D sufficiently large (which is valid as $D \propto e^N$, N the number of degrees of freedom), such that $\mathcal{O}(C(\lambda, t)/\sqrt{D})$ can be neglected and thus

$$\|\hat{P}_1 \psi_t\|^2 \approx 1 - \frac{d_2}{D} + \frac{1}{\pi(\lambda t)^3}, \quad (6.95)$$

$$\|\hat{P}_2 \psi_t\|^2 \approx \frac{d_2}{D} - \frac{1}{\pi(\lambda t)^3}. \quad (6.96)$$

Now we argue that these are right moving and thus satisfy (5.4). This can easily be seen as for $t_2 \geq t_1$, with t_1 and t_2 sufficiently large,

$$\|\hat{P}_2 \psi_{t_1}\|^2 \leq \|\hat{P}_2 \psi_{t_2}\|^2 \quad (6.97)$$

⁴⁶As a technical detail one has to require that all higher moments of $\sqrt{D}\hat{H}$ are bounded (see [93]).

holds. This yields a WSL, which reads

WSL (2x2): Let $\mathcal{H}_{\text{mc}} = \mathcal{H}_1 \oplus \mathcal{H}_2$ be a decomposition of the energy shell, let $\hat{H}$ be a Wigner type matrix fulfilling the assumptions (6.91) and let $\psi_0 \in \mathbb{S}(\mathcal{H}_1)$. Then for typical $\hat{H}$, $t_1 \leq t_2$ with $t_1, t_2 \gg \lambda^{-1}$ and sufficiently large D

$$\|P_1\psi_t\|^2 = 1 - \frac{d_2}{D} + \frac{1}{\pi(\lambda t)^3}, \quad (6.98)$$

$$\|P_2\psi_t\|^2 = \frac{d_2}{D} - \frac{1}{\pi(\lambda t)^3} \quad (6.99)$$

are a family of RMDs.

6.3.2. WSL for three Macrospace

Now consider the setting with three subspaces, more precisely $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3$ with dimension $D = d_1 + d_2 + d_3 = (1 + \lambda + \lambda^2)d$, where $\lambda > 0$ is a small parameter. Again $\mathcal{H}_3 = \mathcal{H}_{\text{eq}}$ and thus one can think of $\mathcal{H}_1 \oplus \mathcal{H}_2 = \mathcal{H}_{\text{neq}}$ as the non-equilibrium subspace. The variance matrix reads

$$S = (S_{ij}) = \begin{pmatrix} S_{11} & S_{12} & 0 \\ S_{21} & S_{22} & S_{23} \\ 0 & S_{32} & S_{33} \end{pmatrix} \quad (6.100)$$

where

$$\begin{aligned} S_{11} &= \frac{1}{(1 + \lambda + \lambda^2)D} \frac{1}{\lambda^2} E_{d_1, d_1} & S_{12} &= S_{21}^* = \frac{1 + \lambda}{(1 + \lambda + \lambda^2)D} E_{d_1, d_2} \\ S_{22} &= \frac{1 - \lambda^3}{\lambda(1 + \lambda + \lambda^2)D} E_{d_2, d_2}, & S_{23} &= S_{32}^* = \frac{\lambda}{(1 + \lambda + \lambda^2)D} E_{d_2, d_3} \\ S_{33} &= \frac{1 + \lambda}{(1 + \lambda + \lambda^2)D} E_{d_3, d_3} \end{aligned}$$

and the blocks with zeroes are adequately sized. Moreover, there is an assumption on the moments of the matrix elements of $\hat{H}$ (see [93]).

We are now interested if the weights with initial states in $\mathcal{H}_1$ or $\mathcal{H}_2$ yield a family of right moving distributions. For $\psi_0 \in \mathbb{S}(\mathcal{H}_3)$ we just settle with the fact that it will stay in that subspace. According to [93, Thm.2.10] the weights are given with very high probability for $\psi_0 \in \mathbb{S}(\mathcal{H}_1)$ by

$$\|\hat{P}_1\psi_t\|^2 = \frac{d_1}{D} + \frac{1}{\pi(\lambda t)^3} (1 + o(1)) + \mathcal{O}(C(\lambda, t)/\sqrt{D}), \quad (6.101)$$

$$\|\hat{P}_2\psi_t\|^2 = \frac{d_2}{D} + \frac{3}{\pi(\lambda t)^3}(1 + o(1)) + \mathcal{O}(C(\lambda, t)/\sqrt{D}), \quad (6.102)$$

$$\|\hat{P}_3\psi_t\|^2 = \frac{d_3}{D} - \frac{4}{\pi(\lambda t)^3}(1 + o(1)) + \mathcal{O}(C(\lambda, t)/\sqrt{D}) \quad (6.103)$$

and for $\psi_0 \in \mathbb{S}(\mathcal{H}_2)$ by

$$\|\hat{P}_1\psi_t\|^2 = \frac{d_1}{D} + \frac{3}{\pi\lambda^2 t^3}(1 + o(1)) + \mathcal{O}(C(\lambda, t)/\sqrt{D}), \quad (6.104)$$

$$\|\hat{P}_2\psi_t\|^2 = \frac{d_2}{D} + \frac{1 - 3\lambda}{\pi(\lambda t)^3}(1 + o(1)) + \mathcal{O}(C(\lambda, t)/\sqrt{D}), \quad (6.105)$$

$$\|\hat{P}_3\psi_t\|^2 = \frac{d_3}{D} - \frac{1}{\pi(\lambda t)^3}(1 + o(1)) + \mathcal{O}(C(\lambda, t)/\sqrt{D}). \quad (6.106)$$

Again, $o(1)$ denotes a quantity vanishing in the limit $t \rightarrow \infty$, $\lambda \rightarrow 0$, and $t\lambda \rightarrow \infty$, and $C(\lambda, t)$ is a constant depending only on its arguments. Now we consider only cases where $t \gg 1/\lambda$ and D large enough such that $\mathcal{O}(C(\lambda, t)/\sqrt{D})$ is negligible. Further in such a limit $o(1)$ is small compared to one. We now derive a WSL by showing that the weights above in the just stated cases are RMDs. We use similar approximations as in the last section to neglect the $o(1)$ and $\mathcal{O}(C(\lambda, t)/\sqrt{D})$ contributions.

The right moving condition (5.4) needs to be checked for $\nu' = 2$ and $\nu' = 3$; for $\nu' = 1$ it trivially holds due to unitarity. Further the initial state can be in different subspaces. Hence we will also make a distinction there. In each case we consider sufficiently large times $t_1, t_2 \geq 0$, such that we can apply [93, Thm.2.10], where $t_2 \geq t_1$.

Let $\nu' = 2$, then

$$\|\hat{P}_2\psi_{t_1}\|^2 + \|\hat{P}_3\psi_{t_1}\|^2 \leq \|\hat{P}_2\psi_{t_2}\|^2 + \|\hat{P}_3\psi_{t_2}\|^2 \quad (6.107)$$

which is equivalent to

$$\|\hat{P}_1\psi_{t_2}\|^2 \leq \|\hat{P}_1\psi_{t_1}\|^2, \quad (6.108)$$

because $\sum_{\nu=1}^3 \|\hat{P}_\nu\psi_t\|^2 = 1$. For $\psi_0 \in \mathbb{S}(\mathcal{H}_1)$, using [93, Thm.2.10], we have with very high probability

$$\|\hat{P}_1\psi_t\|^2 \approx \frac{d_1}{D} + \frac{1}{\pi(\lambda t)^3} \quad (6.109)$$

and one can by a quick calculation see that the above relation indeed holds.

For $\psi_0 \in \mathbb{S}(\mathcal{H}_2)$ one gets with very high probability

$$\|\hat{P}_1\psi_t\|^2 \approx \frac{d_1}{D} + \frac{3}{\pi\lambda^2 t^3}, \quad (6.110)$$

which then yields the same result. For $\psi_0 \in \mathbb{S}(\mathcal{H}_3)$ the weights are given with very

high probability by

$$\|\hat{P}_1\psi_t\|^2 \approx \frac{d_1}{D} - \frac{4}{\pi\lambda t^3} \quad (6.111)$$

and one finds that the condition is violated. This makes sense, because $\mathcal{H}_3$ is the equilibrium subspace and therefore the wave function stays in it.

For $\nu' = 3$ the right moving condition (5.4) reads for $t_1 \leq t_2$ and t_1, t_2 sufficiently large

$$\|\hat{P}_3\psi_{t_1}\|^2 \leq \|\hat{P}_3\psi_{t_2}\|^2. \quad (6.112)$$

.

For $\psi_0 \in \mathbb{S}(\mathcal{H}_1)$ the weights read with very high probability

$$\|\hat{P}_3\psi_t\|^2 \approx \frac{d_3}{D} - \frac{4}{\pi(\lambda t)^3} \quad (6.113)$$

and one can easily see that they fulfill the above condition. The same is true for $\psi_0 \in \mathbb{S}(\mathcal{H}_2)$, while as before for $\psi_0 \in \mathbb{S}(\mathcal{H}_3)$, the right moving condition is violated. Again this is, because the initial state lies already in thermal equilibrium and has almost no chance to go anywhere else.

With all this we state the WSL as our final result:

WSL for Wigner Type Matrices II: Let $\mathcal{H}_{\text{mc}} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3$ be a decomposition of the energy shell, let $\hat{H}$ be a Wigner type matrix fulfilling the assumptions just stated and let $\psi_0 \in \mathbb{S}(\mathcal{H}_\nu)$ with $\nu = 1, 2$, then for typical $\hat{H}$, $t \gg 1/\lambda$ and large enough D the weights $\|\hat{P}_\nu\psi_t\|^2$ above with $\nu = 1, 2, 3$ are a family of RMDs.

7. General Approaches

In Section 7.1 it is shown that the formalism used above can be extended to a more general class of random Hamiltonians, also allowing to treat systems with a more local interaction structure. Although not treatable at an analytical level at this moment, it builds the foundation for possible research in the future. Another approach to treat the effective dynamics is sketched in Section 7.2.

7.1. General Approach for Wigner Matrix Models

Relevant to the problem of entropy increase presented here are the macroscopic weights $||\hat{P}_\nu \psi_t||^2$ and the current $J_{\nu\nu'}^{\psi_0}(t)$. Above we discussed examples for the typical behavior of a Hamiltonian $\hat{H}$ being modeled by a Wigner matrix. However this is a rather unrealistic case for physical systems, because it does not take the locality of interactions into account. It mimics the behavior of a system where every particle interacts in the same way with every other particle independent whether they are far away or close to each other (this is also referred to as a mean field model). As interaction is key for thermalization [31], the mean field interaction leads to ultrafast thermalization. Another case that we discussed added more structure to the Hamiltonian $\hat{H}$ via a more general variance profile. This leads into the direction of more realistic physical behavior and also to more realistic thermalization times [93]. However, the number of macro spaces is limited to two or three.

Let $\hat{H} = (h_{ij})$ be a Wigner matrix model with ordered random eigenvalues $E_1 \leq \dots \leq E_D$ and

$$\mathbb{E}h_{ij} = 0 \quad \text{and} \quad \mathbb{E}|h_{ij}|^2 = S_{ij} \quad (7.1)$$

where S_{ij} is the variance matrix. Using residue calculus

$$e^{-i\hat{H}t} = \frac{1}{2\pi i} \oint_{\gamma} dz e^{-itz} G(z), \quad (7.2)$$

$$\hat{H} = \frac{1}{2\pi i} \oint_{\gamma} dz z G(z), \quad (7.3)$$

where γ denotes the respective contour enclosing the spectrum of $\hat{H}$ and the resolvent

7. General Approaches

$G(z)$ for spectral parameter $z = E + i\eta$ with $\eta > 0$ and is defined as

$$G(z) := (\hat{H} - z)^{-1}. \quad (7.4)$$

One can write the weights $p_\nu(t)$ and the current $J_{\nu\nu'}^{\psi_0}(t)$ for $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$ as

$$||\hat{P}_\nu \psi_t||^2 = \frac{1}{(2\pi i)^2} \oint_{\gamma_1} \oint_{\gamma_2} dz_1 dz_2 e^{it(z_1 - z_2)} \langle \psi_0 | G(z_1) \hat{P}_\nu G(z_2) | \psi_0 \rangle, \quad (7.5)$$

$$J_{\nu\nu'}^{\psi_0}(t) = 2\text{Im} \frac{1}{(2\pi i)^3} \oint_{\gamma_1} \oint_{\gamma_2} \oint_{\gamma_3} dz_1 dz_2 dz_3 e^{it(z_1 - z_3)} z_2 \quad (7.6)$$

$$\times \langle \psi_0 | G(z_1) \hat{P}_\nu G(z_2) \hat{P}_{\nu'} G(z_3) | \psi_0 \rangle \quad (7.7)$$

with γ_1, γ_2 and γ_3 , the respective contours enclosing the spectrum of $\hat{H}$. Therefore the goal is to approximate

$$\langle \psi_0 | G(z_1) \hat{P}_\nu G(z_2) | \psi_0 \rangle, \quad (7.8)$$

$$\langle \psi_0 | G(z_1) \hat{P}_\nu G(z_2) \hat{P}_{\nu'} G(z_3) | \psi_0 \rangle \quad (7.9)$$

by a deterministic quantity and then carry out the contour integration afterwards. This can be done by using so called multi-resolvent laws. Motivated by proving the ETH and related thermal properties of many-particle systems, these have been developed in the last few years for Wigner matrices [63, 64, 66, 59, 60], deformed Wigner matrices [61, 62] and other Wigner matrix models [94]. There it turned out that products of the form

$$G(z_1) B_1 G(z_2) B_2 \cdots B_{k-1} G(z_k) \quad (7.10)$$

with deterministic matrices B_i and $z_l = E_l + i\eta_l$ play a decisive role. There are two senses under which the convergence can be understood and the one relevant for us is⁴⁷, that for fixed vectors $\mathbf{x}, \mathbf{y} \in \mathbb{C}^D$

$$\langle \mathbf{x}, G(z_1) B_1 G(z_2) B_2 \cdots B_{k-1} G(z_k) \mathbf{y} \rangle \quad (7.11)$$

approaches its deterministic approximation for large D with very high probability.

It is a well known fact that for large D the resolvent $G(z)$ of a Wigner matrix $\hat{H}$, typically concentrates around a deterministic value $m = m(z)$ (see, e.g., [96, 64]). It allows for instance to compute the density of eigenvalues in certain regimes by solving the quadratic equation

$$1 + (z + m)m = 0. \quad (7.12)$$

⁴⁷One can also consider typical initial states, see [65]. That does not change the result in any drastic manner.

Let us just mention that m is related to the eigenvalue distribution via a Stieltjes transform (see [65, 91, 95] for details).

This is also the case for random matrices, which allow more structure in the variance matrix S (also for $\mathbb{E}h_{ij} \neq 0$, but this is not important here). Then the resolvent $G(z)$ is approximated by a deterministic object $M(z)$ which is the solution to the vector-Dyson-equation (VDE)

$$1 + (z + S[M])M = 0 \quad (7.13)$$

under the constraint $\text{Im}M = \frac{1}{2i}(M - M^*) > 0$ with variance matrix S .

Now for other matrices, e.g., Wigner-type matrices, which are Wigner matrices with possibly centered entries and a general variance profile $S_{ij} = \mathbb{E}|h_{ij}|^2$ the approximation is given by $M(z) = \text{diag}(\mathbf{m})$, i.e., a matrix that carries all the entries of the vector $\mathbf{m}(z) = (m_j(z))$ with $j = 1, \dots, D$ along the diagonal [94]; for other Wigner ensembles see [91]. Then the VDE explicitly reads

$$1 + zm_j(z) + \sum_{k=1}^D S_{jk}m_k(z)m_j(z) = 0 \quad (7.14)$$

Our interest are the typical values of (7.8) and (7.9) and therefore we “only” need two - and three resolvent laws for any initial state $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$. That is however highly non-trivial as for realistic random matrix models the variance matrix leads to a highly non-linear VDE. The VDE has to be solved in order to find the values for $M(z)$, which then allows to find an approximation for (7.8) and (7.9). But that is not the end of the story. The VDE is needed to find the distribution for the eigenvalues, in particular deterministic approximations for $G(z)$, but not for products of the form (7.8) and (7.9). Let us briefly sketch how this looks like for (7.8) in our case (for more details see [93] and the cited references therein). One can show that for $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu})$ and large enough D

$$\langle \psi_0 | G(z_1) \hat{P}_{\nu} G(z_2) | \psi_0 \rangle \approx \langle \psi_0 | M(z_1, \hat{P}_{\nu}, z_2) | \psi_0 \rangle \quad (7.15)$$

holds with very high probability. The deterministic approximation $M(z_1, \hat{P}_{\nu}, z_2)$ can be computed using the inverse of the variance matrix S and $M(z_1), M(z_2)$, which are solutions to the VDE. We can not state all the details here, so we refer to [93, Eq.3.6]. The take home message is that a typical value for (7.8) and (7.9) relies on solving complicated (possibly) non-linear equations.

Assume for the moment that for D large enough the typical solutions $M(z_1, \hat{P}_{\nu}, z_2)$ for (7.8) and $M(z_1, \hat{P}_{\nu}, z_2, \hat{P}_{\nu'}, z_3)$ for (7.9) have been found. Then the typical weights and currents read

$$||\hat{P}_{\nu}\psi_t||^2 = \frac{1}{(2\pi i)^2} \oint_{\gamma_1} \oint_{\gamma_2} dz_1 dz_2 e^{it(z_1 - z_2)} \langle \psi_0 | M(z_1, \hat{P}_{\nu}, z_2) | \psi_0 \rangle, \quad (7.16)$$

$$J_{\nu\nu'}^{\psi_0}(t) = 2\text{Im} \frac{1}{(2\pi i)^3} \oint_{\gamma_1} \oint_{\gamma_2} \oint_{\gamma_3} dz_1 dz_2 dz_3 e^{it(z_1 - z_3)} z_2 \quad (7.17)$$

$$\times \langle \psi_0 | M(z_1, \hat{P}_\nu, z_2, \hat{P}_{\nu'}, z_3) | \psi_0 \rangle. \quad (7.18)$$

From thereon one would have to depending on the precise form of the M 's use integration techniques. It is known, that M is function of $m(z_i)$ with $i = 1, 2, 3$, where the $m(z_i)$ are solutions to the VDE [93, Sec.3.1]. Notice that the current also has a factor z_2 , which leads to the following simplification (as first calculations have shown, not published here or elsewhere): let $n \in \mathbb{N}$, $m(z)$ and γ a suitable contour. Then

$$\frac{1}{2\pi i} \oint_{\gamma} dz z m^n(z) = 1 \quad (7.19)$$

for $n = 2$ and zero else (which can be seen from [93, App.A.1] using the rule of l'Hospital).

Summarizing the above steps for future research, the procedure to find deterministic approximations for the weights and currents could look like this:

- (1) define a random Hamiltonian with variance profile $S_{ij} = \mathbb{E}|h_{ij}|^2$, that models the relevant physical properties of the system, such as locality of interactions.
- (2) find a deterministic approximation for (7.8) and (7.9) by solving the non-linear VDE and the respective equations for $M(z_1, \hat{P}_\nu, z_2, \hat{P}_{\nu'}, z_3)$ (see [93, Sec.4]).
- (3) Carry out the contour integrals that appear in $||\hat{P}_\nu \psi_t||^2$ and $J_{\nu\nu'}^{\psi_0}(t)$.

Clearly, every step of the procedure is highly non-trivial and invites for trade-offs between mathematical rigor and modelling the physically relevant characteristics of the system. In case of the latter, numerical simulations (such as solutions to the VDE for physically more realistic variance profiles) could yield deterministic approximations to (7.8) and (7.9).

7.2. Effective Dynamics

Let us discuss another approach towards computing typical weights and currents following [288]. Suppose $(\{\mathcal{H}_\nu\}, \hat{H}, \psi_0)$ is a reasonable choice, where we consider the subspaces as fixed, while the entries of $\hat{H}$ are sampled according to some probability measure $\mathbb{P}_{\hat{H}}$ and $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$ is also sampled according to some probability measure $\mathbb{P}_{\psi_0}$. In general we speak of Hamiltonians $\hat{H}$ that allow for “nice statistics”.

Let $\mathcal{H} = \oplus_\nu \mathcal{H}_\nu$ be a decomposition of $\mathcal{H}$ with $\dim \mathcal{H} = D$; let $\mathcal{N}$ denote the set of macro states ν . Let $\hat{H} = \sum_n E_n |\phi_n\rangle\langle\phi_n|$ be a Hamiltonian, such that the weights

can be split up into a time-independent and time dependent part

$$||\hat{P}_\nu \psi_t||^2 = \sum_n |\langle \psi_0 | \phi_n \rangle|^2 \langle \phi_n | \hat{P}_\nu | \phi_n \rangle \quad (7.20)$$

$$+ \sum_{n \neq m} \langle \psi_0 | \phi_n \rangle \langle \phi_m | \psi_0 \rangle \langle \phi_n | \hat{P}_\nu | \phi_m \rangle e^{it(E_n - E_m)}. \quad (7.21)$$

A simple first step might be to consider sampling initial states. A natural probability measure is the uniform measure on the unit sphere of the subspace of initial macro states. Then one finds for $\psi_0 \sim u_{\mathbb{S}(\mathcal{H}_{\nu_0})}$, that

$$\mathbb{E}_{u_{\mathbb{S}(\mathcal{H}_{\nu_0})}} ||\hat{P}_\nu \psi_t||^2 = \frac{1}{d_{\nu_0}} \text{tr}(\hat{P}_{\nu_0} e^{i\hat{H}t} \hat{P}_\nu e^{-i\hat{H}t}). \quad (7.22)$$

More general one can assume that initial states are sampled according to the GAP measure (GAP measures are quantum analogs of probability distributions of classical micro states in thermal equilibrium, see Part III). That is for $\psi_0 \sim \text{GAP}_{\hat{\rho}_{\nu_0}}$ one has

$$w_\nu(t) := \mathbb{E}_{\text{GAP}_{\hat{\rho}_{\nu_0}}} ||\hat{P}_\nu \psi_t||^2 = \text{tr}(\hat{\rho}_{\nu_0} e^{i\hat{H}t} \hat{P}_\nu e^{-i\hat{H}t}). \quad (7.23)$$

Note that the uniform measure u_ν is a special instance of the GAP measure, namely $u_\nu = \text{GAP}_{\hat{\rho}_\nu}$ for $\hat{\rho}_\nu = \hat{P}_\nu / d_\nu$.

We aim at an approximation of $w_\nu(t)$ through $W_\nu(t)$. The basic idea is to consider random Hamiltonians $\hat{H}$ and the statistical distribution of the eigenvalues and eigenvectors in order to replace sums that appear in (7.20) by integrals. Among those distributions is the density of states $\Omega(E)$. Then for large enough D ,

$$\frac{1}{D} \sum_n \rightarrow \int dE \Omega(E). \quad (7.24)$$

We will explain now in detail how the other statistical distribution of $\hat{H}$ come into play. Let $I_{\text{mc}} = [E - \Delta E, E]$ denote as usual the micro-canonical energy intervall. Let $\#Y$ denote the counting measure, i.e., the number of elements in the set Y .

Let us start with the density of states. It is defined as follows:

$$\Omega(E) := \frac{\#\{n : E_n \in I_{\text{mc}}\}}{\Delta E D} = \frac{1}{D \Delta E} \sum_{n: E - \Delta E \leq E_n \leq E} \delta(E - E_n). \quad (7.25)$$

That is $\Omega(E)$ describes the actual empirical distribution of the eigenvalues⁴⁸. In (7.20)

⁴⁸As we look for typicality statements, keep in mind that these connect empirical distributions with theoretical distributions (see Section 3).

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also $\langle \phi_n | \hat{P}_\nu | \phi_n \rangle$ appear. As the eigenvectors are random their empirical distribution is given by

$$\eta_E(A) := \frac{\#\{n : E_n \in I_{\text{mc}} \text{ and } (\langle \phi_n | \hat{P}_\nu | \phi_n \rangle)_\nu \in A\}}{\Delta E D} \quad (7.26)$$

with $A \subseteq \text{Sim}$, where Sim is the $\mathcal{N}$ -simplex

$$\text{Sim} = \left\{ \mathbf{f} : \mathcal{N} \rightarrow [0, 1] : \sum_{\nu \in \mathcal{N}} f_\nu = 1 \right\}. \quad (7.27)$$

Here $\mathbf{f}$ is a $\#\mathcal{N}$ dimensional vector with components $f_\nu = \langle \phi_n | \hat{P}_\nu | \phi_n \rangle$. That is, the distribution $\eta_E(A)$ is given through the distribution of the points $(\langle \phi_n | \hat{P}_\nu | \phi_n \rangle)_\nu$ on A (for those eigenvectors with eigenvalue in I_{mc}). In particular for $\psi_0 \sim \text{GAP}_{\hat{\rho}_{\nu_0}}$ we have $f_{\nu_0} = \langle \phi_n | \hat{\rho}_{\nu_0} | \phi_n \rangle$.

With this the time independent part of (7.20) is given by⁴⁹

$$\frac{1}{d_{\nu_0}} \sum_n \langle \phi_n | \hat{P}_{\nu_0} | \phi_n \rangle \langle \phi_n | \hat{P}_\nu | \phi_n \rangle \approx \frac{D}{d_{\nu_0}} \int_{\mathbb{R}} dE \Omega(E) \int_{\text{Sim}} \eta_B(df) f_{\nu_0} f_\nu. \quad (7.28)$$

For the time dependent part another distribution has to be defined. Let

$$\mathcal{C} := \left\{ \mathbf{z} : \mathcal{N} \rightarrow \mathbb{C} : \sum_{\nu \in \mathcal{N}} z_\nu = 0 \right\}, \quad (7.29)$$

with $\mathbf{z}$ the $\#\mathcal{N}$ -dimensional vector with components $z_\nu = \sqrt{D} \langle \phi_n | \hat{P}_\nu | \phi_m \rangle$ and $E, E' \in \mathbb{R}$ with $I'_{\text{mc}} = [E' - \Delta E', E']$. Then the empirical distribution of z_ν is for $A \subseteq \mathcal{C}$ given by

$$\zeta_{E,E'}(A) = \frac{\#\{(n, m) : E_n \in I_{\text{mc}}, E_m \in I'_{\text{mc}}, (\sqrt{D} \langle \phi_n | \hat{P}_\nu | \phi_m \rangle)_\nu \in A\}}{\#\{(n, m) : E_n \in I_{\text{mc}}, E_m \in I'_{\text{mc}}\}}. \quad (7.30)$$

Approximating the time-dependent part in the same way as the time independent part we get the final result

$$W_\nu(t) \approx \frac{D}{d_{\nu_0}} \int_{\mathbb{R}} dE \Omega(E) \int_{\text{Sim}} \eta_E(df) f_{\nu_0} f_\nu \quad (7.31)$$

$$+ \frac{D}{d_{\nu_0}} \int_{\mathbb{R}} dE dE' \Omega(E) \Omega(E') e^{it(E-E')} \int_{\mathcal{C}} \zeta_{E,E'}(d\mathbf{z}) z_{\nu_0}^* z_\nu. \quad (7.32)$$

Similar considerations can be made for the current (5.6). As this involves more differ-

⁴⁹Note that we consider non-degenerate Hamiltonians $\hat{H}$, such that the replacement of sums through integrals is well posed.

ent contributions from the overlaps of the energy eigenvectors with the projectors $\hat{P}_\nu$ it is more tedious and will not be stated here (see [288]).

The upshot is that the time evolution of the weights (and the current) can be effectively described using statistical distributions, such as η_E and $\xi_{E,E'}$.

The goal is to derive theoretical distributions, that is “smoothed” out versions of the empirical distributions η_E and $\xi_{E,E'}$ for random Hamiltonians $\hat{H}$. This would be done in such a way that these smoothed out versions would be the *typical* distributions with respect to the distribution of $\hat{H}$. For instance:

$$\mathbb{P}_{\hat{H}} \{ |\eta_E - \eta(E)| < \delta \} \geq 1 - \varepsilon \quad (7.33)$$

with $\delta, \varepsilon > 0$ and δ possibly depending on ε or the dimension D . That is for suitable δ, ε , the empirical distribution η_E is close to the theoretical distribution $\eta(E)$. Or in other words $\eta(E)$ is typical with respect to $\mathbb{P}_{\hat{H}}$. As pointed out in [288] this seems possible for GUE Hamiltonians yielding (again) a similar behavior as for Wigner matrices, but for realistic cases such a statement is currently out of reach.

8. Second Law in Boltzmann-Bohm Framework

We now take foundational issues arising from the measurement problem discussed in Section 3.3.1 into account. The appearance of macroscopic superpositions in the context of the BQF has been hinted at in [128, 136, 9], but not worked out more closely. Here we address these issues within Bohmian mechanics (BM), in particular in Section 8.1 we propose a novel version for the second law and sketch some ideas for a more general Bohmian version of quantum statistical mechanics. Let us stress that BM explains the standard axioms, such as the Born rule or the collapse of the wave function. In particular BM solves the measurement problem by relying on a particle ontology (see, e.g., [172]). Finally, in Section 8.2 we discuss a version of the second law in the Boltzmann-Bohm framework.

8.1. Boltzmann-Bohm Second Law

The WSL and SSL are well posed in the standard framework of quantum mechanics. However due to superpositions of macroscopic entropy states, we have to appeal to quantum theory without observers. Here we discuss the Bohmian approach connecting it to the concepts of the BQF introduced above in Part I and call it **Bohm-Boltzmann Framework (BBF)**. We define a macro state as follows

$$\nu_t = \nu(Q(t), \psi_t) \quad (8.1)$$

as consisting of the wave function ψ_t and $Q(t)$ being the particle configuration. Now with respect to the measurement problem discussed in Section 3.3.1 there is a fact about the actual particle positions and thus also about the actual macroscopic entropy value, although the wave function is still in a superposition. That is for our example in Section 3.3.1

$$\psi = c_{\text{eq}}\psi_{\text{eq}} + c_{\text{neq}}\psi_{\text{neq}} \quad (8.2)$$

there is a corresponding configuration $Q = Q_{\text{eq}}$ or $Q = Q_{\text{neq}}$ having probability distribution $Q \sim |\psi|^2$ (compare with (3.35)), which chooses one of the macroscopically different macro states, here eq or neq. Indeed this happens if the wave functions do

not overlap much in configuration space, i.e.,

$$\text{supp}(\psi_{\text{eq}}) \cap \text{supp}(\psi_{\text{neq}}) \approx \emptyset. \quad (8.3)$$

In that case there is an actual entropy value, i.e.,

$$S(Q, \psi) = S(\text{eq}) \iff Q \in \text{supp}(\psi_{\text{eq}}). \quad (8.4)$$

There is however a subtlety as Q does not always select a unique macro state ν and therefore a unique $S_{\text{QB}}(\nu)$. Such artificial examples can be constructed (e.g. ideal gas), but for practical purposes it is believed to work.

With all that being said, the second law of thermodynamics for closed quantum system proposed in a Bohmian setting builds on conjecture 4.1 and reads

Boltzmann-Bohm Second Law: For a reasonable choice of Hamiltonian H , decomposition $\mathcal{H} = \bigoplus_{\nu} \mathcal{H}_{\nu}$, initial macro state $\nu_0(Q(0), \psi_0)$ with initial wave function $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$ and initial configuration Q_0 . Then with probability close to one, $S_{\text{B}}(\nu_t)$ is non-decreasing with time, except for infrequent, shallow, and short lived valleys, up to a time T , until it reaches the thermal equilibrium value $S_{\text{B}}(\nu_{\text{eq}})$, where T is the time scale of reaching MATE. Moreover, $S_{\text{B}}(\nu_{\text{eq}})$ stays at that value for a very long time.

Remark 8.1.1. We formulated a version of the second law for Bohmian mechanics. As there are other proposals solving the measurement problem, such as the GRW-theory or the many worlds theory (see, e.g., [83, 113]) it would certainly be of interest to see how the second law or the BQF in general looks like in these cases. $\diamond$

8.2. Bell Second Law

Since $Q(t) \sim |\psi_t|^2$, the evolution of the macrostate ν_t , i.e., $(\nu_t)_{t \in \mathbb{R}}$, will be a stochastic jump process on the set of macrostates, for which its Markovization can be approximated by a Bell process [17]. To apply this to our setting, we briefly explain the necessary ingredients of the Bell process [13].

A Bell process is a Markovian jump process $(Y_t)_{t \in \mathbb{R}}$ on a lattice $\mathcal{Y}$ with jump rates $y \rightarrow y'$ given by

$$\sigma_t(y|y') = \frac{[2\text{Im}\langle\psi_t|\hat{P}(y)H\hat{P}(y')|\psi_t\rangle]^+}{\langle\psi_t|\hat{P}(y')|\psi_t\rangle}, \quad (8.5)$$

with $x^+ = \max(x, 0)$. The state ψ_t follows the Schrödinger evolution and $\hat{P}(y)$ is a projection onto the subspace $\mathcal{H}_y \subseteq \mathcal{H}$, where $\mathcal{H} = \bigoplus_{y \in \mathcal{Y}} \mathcal{H}_y$ [13]. It has the following properties:

(i) At every time t , the distribution of Y_t is

$$\mathbb{P}(Y_t = y) = \langle \psi_t | \hat{P}(y) | \psi_t \rangle. \quad (8.6)$$

(ii) The net probability current between y' and y ,

$$J_{yy'} = \sigma_t(y|y')\mathbb{P}(Y_t = y') - \sigma_t(y'|y)\mathbb{P}(Y_t = y) \quad (8.7)$$

agrees with the quantum expression for the probability current

$$2\text{Im}\langle \psi | \hat{P}(y) H \hat{P}(y') | \psi \rangle. \quad (8.8)$$

We will now apply this to our setting: $(\nu_t)_{t \in \mathbb{R}}$ defines a jump process on $\mathcal{N}$. This means, that the rate for a transition from ν' to ν is given by

$$\sigma_t(\nu|\nu') = \frac{\left[J_{\nu\nu'}^{\psi_0}(t) \right]^+}{\|\hat{P}_{\nu'}\psi_t\|^2}, \quad (8.9)$$

while the transition rates from ν to ν' are given by

$$\sigma_t(\nu'|\nu) = \frac{\left[J_{\nu'\nu}^{\psi_0}(t) \right]^+}{\|\hat{P}_\nu\psi_t\|^2}. \quad (8.10)$$

Of course in order for entropy to increase, there should be more transitions from a lower dimensional ν to a higher dimensional ν' . This allows us to formulate a version of the second law:

Bell Second Law (BSL): For a reasonable choice of $\hat{H}$, decomposition $\mathcal{H}_{\text{mc}} = \bigoplus_\nu \mathcal{H}_\nu$, initial macro state ν_0 , $\psi_0 \in \mathbb{S}(\mathcal{H}_{\nu_0})$ and two macro states ν, ν' with $d_{\nu'} > d_\nu$, there are overwhelmingly more transitions from ν to ν' , i.e.,

$$\sigma_t(\nu|\nu') \ll \sigma_t(\nu'|\nu) \quad (8.11)$$

for $t \in [0, T]$, where T is the time scale of reaching MATE.

Note that if the BSL holds, as a consequence the Bell process $(\nu_t)_{t \in [0, T]}$ on $\mathcal{N}$ has increasing $S_{\text{QB}}(\nu_t)$ for $t \in [0, T]$. As a reasonable choice we consider again (as in Section 6.2) a Wigner matrix $\hat{H}$.

Using (6.55) and (6.15) we can compute (8.9) and (8.10). Let $d_{\nu'} > d_\nu$ and let $\nu = \nu_0$. We now show that there are more transitions from ν to ν' than the other way around. Recall that $x^+ = \max(0, x)$ denotes the positive and $x^- = \min(0, x)$ the negative part of x .

First we compute

$$\left[J_{\nu'\nu}^{\psi_0}(t) \right]^+ = \left[-\frac{4d_{\nu'}}{D} \varphi_1(t) \varphi_2(t) \right]^+ = -4\frac{d_{\nu'}}{D} (\varphi_1(t) \varphi_2(t))^- \quad (8.12)$$

and using $J_{\nu\nu'}^{\psi_0}(t) = -J_{\nu'\nu}^{\psi_0}(t)$, which implies $[J_{\nu'\nu}^{\psi_0}(t)]^+ = [J_{\nu\nu'}^{\psi_0}(t)]^-$, we get

$$\left[J_{\nu\nu'}^{\psi_0}(t) \right]^- = -4\frac{d_{\nu'}}{D} (\varphi_1(t) \varphi_2(t))^+. \quad (8.13)$$

For the weights (6.15) we immediately obtain

$$\|\hat{P}_{\nu'} \psi_t\|^2 = \frac{d_{\nu'}}{D} (1 - \varphi_1^2(t)), \quad (8.14)$$

$$\|\hat{P}_{\nu} \psi_t\|^2 = \frac{d_{\nu}}{D} (1 - \varphi_1^2(t)) + \varphi_1^2(t) \quad (8.15)$$

and hence for sufficiently large enough times $t \in [0, T]$, such that $\varphi_1^2(t) \approx 0$ (reasonable assumption, see Figure 6.1), we get

$$\frac{\sigma_t(\nu'|\nu)}{\sigma_t(\nu|\nu')} \approx \frac{d_{\nu'}}{d_{\nu}} \frac{\left[J_{\nu\nu'}^{\psi_0}(t) \right]^-}{\left[J_{\nu\nu'}^{\psi_0}(t) \right]^+} \approx \frac{d_{\nu'}}{d_{\nu}} \frac{(\varphi_1(t) \varphi_2(t))^+}{(\varphi_1(t) \varphi_2(t))^-} \gg 1. \quad (8.16)$$

Here the last step follows from $d_{\nu'} > d_{\nu}$ and the fact that the positive part of $\varphi_1(t) \varphi_2(t)$ is much bigger than the negative part for suitable t (see Figure 6.3).

As a consequence the Bell process $(\nu_t)_{t \in [0, T]}$ has increasing entropy $S_{\text{QB}}(\nu_t)$.

Part III.

Boltzmannian Quantum Framework for Subsystems

9. Thermal Equilibrium of Subsystems

The main aim of this part is to elaborate the content in Appendix 11.2 in more detail and propose an answer to the question raised in Section 1.3: “What justifies the use of ensembles?” One reason given in the literature (see, e.g., [11, 146]) is that they are extremely successful in practice. But that does not answer the question in a satisfying way⁵⁰. Another answer usually given in the literature is to propose principles, such as the principle of equal a priori probabilities (PEP) [281, 212] or the maximum entropy principle (MEP) [152, 11], which yield the thermodynamic ensembles (ultimately these principles are principles, but they are made reasonable by their empirical consequences). Both of these principles have flaws as they rely on an ensemblistic understanding of statistical mechanics. That is instead of asking the *right* question regarding thermal equilibrium, namely

Why is a system in thermal equilibrium?

the following question is asked (see, e.g., [11, 244, 146]):

Given a system in thermal equilibrium. How can one assign a probability distribution over the set of micro states compatible with macroscopic equilibrium given the data one has about the system?

The answer is of course known and given by the canonical distributions, which are derived using the PEP or the MEP. But that does not answer the first question. What does it mean that a system “has” a distribution? Why does data or knowledge play a role for a system being in thermal equilibrium at all?

We do not follow this view and give another reason. The reason why systems are in thermal equilibrium is because that is typical [121, 84, 136, 272]:

Typicality of thermal equilibrium: It is the essential feature of thermal equilibrium that micro states in thermal equilibrium behave like most micro states.

That also answers the second question as we will see below. Thermodynamic ensembles are best understood in terms of typicality (see, e.g., [136, 121]).

⁵⁰Note that this is similar to driving a car. To drive it you don’t need to know how the engine and so on works. But it’s still worthwhile to know [287, Sec.8.2].

In Section 9.1 we introduce the basic setup. Then in Section 10 we recall the well known thermodynamic ensembles, while also presenting the generalized Gibbs ensembles. In Section 9.3 microscopic thermal equilibrium (MITE) is defined and in Section 9.4 the temporal evolution towards MITE.

9.1. State of a Subsystem

We now discuss two ways to assign a state to S , one through density matrices and one through wave functions.

Density Matrix

A common and most general description for a quantum system is given by a density matrix $\hat{\rho}$, a positive, self-adjoint operator on $\mathcal{H}$ with unit trace.

Density matrices arise in at least three ways, either as a **reduced density matrix**, as a **statistical operator** or as a combination of both. A further possibility relies on the conditional wave function known as the conditional density matrix (see, e.g., [81]). Only the first three are relevant for us here.

Suppose the combined system $S \cup B$ is in a state $\hat{\rho}$, where $\hat{\rho}$ is an operator on the total Hilbert space $\mathcal{H} = \mathcal{H}^S \otimes \mathcal{H}^B$. Here $\mathcal{H}^S$ is the Hilbert space of S and $\mathcal{H}^B$ is the Hilbert space of B . Then the state of S is given by the reduced density matrix

$$\hat{\rho}^S = \text{tr}^B \hat{\rho}, \quad (9.1)$$

by tracing out the bath degrees of freedom. Important to note is that if $S \cup B$ is in a pure state, then $\hat{\rho}^S$ can still be mixed. That is a purely quantum phenomenon, due to entanglement between S and B .

Density matrices as statistical operators go back to von Neumann [206] and arise as follows. Suppose a wave function $\Psi \in \mathbb{S}(\mathcal{H})$ is distributed according to some probability measure μ on $\mathbb{S}(\mathcal{H})$. Then the statistical operator is given by

$$\hat{\rho}_\mu = \int_{\mathbb{S}(\mathcal{H})} \mu(d\psi) |\psi\rangle\langle\psi|, \quad (9.2)$$

or stated differently

$$\hat{\rho}_\mu = \mathbb{E} |\Psi\rangle\langle\Psi|, \quad (9.3)$$

that is a mixture of pure states.

Density matrices are useful to compute the statistics of measurement outcomes. Let $\hat{A}$ be a self-adjoint operator, then the probability of finding an outcome $\alpha \in \tilde{B}$

with $\tilde{B} \subseteq \mathbb{R}$ when “measuring $\hat{A}$ ” is

$$\mathbb{P}(\alpha \in \tilde{B}) = \text{tr}(\hat{\rho}_\mu \hat{P}_{\hat{A}}(\tilde{B})), \quad (9.4)$$

where $\hat{P}_{\hat{A}}(\tilde{B})$ is the PVM⁵¹ of $\hat{A}$. Stated differently for $\Psi \sim \mu$, giving it a more individualistic character, one gets with (9.4) and (9.2)

$$\mathbb{P}(\alpha \in \tilde{B}) = \mathbb{E}\langle \Psi | \hat{P}_{\hat{A}}(\tilde{B}) | \Psi \rangle. \quad (9.5)$$

The measurement statistics is thus solely given by the density matrix and the probability measure has “disappeared”. This has severe consequences. First note that different probability measures μ, μ' , can yield the same density matrix $\hat{\rho}_\mu = \hat{\rho}_{\mu'}$ and therefore the same statistics for the outcomes of measurements [81]. This is due to fact that the mapping $\mu \mapsto \hat{\rho}_\mu$ is many-to-one. Consider the following example [287, p.216]: for $\mathcal{H} = \mathbb{C}^2$, the uniform distribution u over $\mathbb{S}(\mathcal{H})$ has density matrix $\hat{\rho}_u = \frac{1}{2}\mathbb{1}$. Let $|\alpha\rangle, |\beta\rangle$ be an ONB of $\mathbb{C}^2$, then the probability distribution

$$\mu' = \frac{1}{2}\delta_{|\alpha\rangle} + \frac{1}{2}\delta_{|\beta\rangle} \quad (9.6)$$

also has density matrix $\hat{\rho}_{\mu'} = \frac{1}{2}\mathbb{1}$. Such distributions are called empirically equivalent. This will also be important later, when we discuss the GAP distribution (see Chapter 10).

As a consequence a measure μ can not be determined experimentally. This is especially interesting as it shows a **limitation to knowledge**. Discussed at several points of this thesis and also again below knowledge plays a key role in certain approaches to statistical mechanics and quantum mechanics. While in these cases knowledge is related to the ignorance of an observer, the result just stated is related to an epistemically inaccessibility and really is what it means: a limitation. There is no way to find out! For more details see [287, Sec. 5.1.4].

Remark 9.1.1. There is an interesting recent result on the limitation to knowledge regarding the quantum state of the universe by Chen and Tumulka [55]. Let Ψ_0 be the initial quantum state of the universe. Assume that its typical in a high-dimensional subspace $\mathcal{H}_{\nu_0} \subset \mathcal{H}$. Then one can (besides other things) show that any particular observation is not able to find out what the initial universal wave function Ψ_0 in $\mathcal{H}_{\nu_0}$ was. $\diamond$

Combining both also leads to a statistical reduced density matrix [287, 81], as now instead of $S \cup B$ being in the state $\hat{\rho}$ it is in the state $\Psi \in \mathbb{S}(\mathcal{H}^S \otimes \mathcal{H}^B)$ with

⁵¹For the general definition see [287, Sec.5.1]. Let us consider a simple case. Let $B \subset \mathbb{R}$ and let $\hat{A}$ be a self-adjoint operator that is diagonalizable, has eigenvalues λ_i and projectors $\hat{\Pi}_i$. Then the PVM is given by $E(B) = \sum_{i:\lambda_i \in B} \hat{\Pi}_i$ and $\hat{A} = \sum_i \lambda_i \hat{\Pi}_i$.

distribution μ on $\mathbb{S}(\mathcal{H}^S \otimes \mathcal{H}^B)$. Then the state of S is given by

$$\hat{\rho}_\Psi^S = \mathbb{E} \operatorname{tr}^B |\Psi\rangle\langle\Psi| = \operatorname{tr}^B \mathbb{E} |\Psi\rangle\langle\Psi|, \quad (9.7)$$

where $\mathbb{E}$ is the expectation with respect to μ ; if not stated otherwise $\mathbb{E}$ will be clear from the context. The probability distribution for measurement outcomes concerning S is given by

$$\mathbb{P}(\alpha \in \tilde{B}) = \operatorname{tr}(\hat{\rho}_\Psi^S \hat{P}_{\tilde{A}}(\tilde{B})) \quad (9.8)$$

with $\alpha \in \tilde{B}$, $\hat{A}$ and $\hat{P}_{\tilde{A}}(\tilde{B})$ as above.

Conditional Wave Function

It is also possible to assign a wave function ψ^S as the state of S . Let $\Psi \in \mathbb{S}(\mathcal{H})$ with $\mathcal{H} = \mathcal{H}^S \otimes \mathcal{H}^B$ and $\dim \mathcal{H} < \infty$. Let $b = \{|b_1\rangle, |b_2\rangle, \dots\}$ be an ONB of $\mathcal{H}^B$. The **conditional wave function** is defined as

$$\psi^S = \frac{\langle b_J | \Psi \rangle_B}{\|\langle b_J | \Psi \rangle_B\|}, \quad (9.9)$$

where $\langle \cdot | \cdot \rangle_B$ denotes the partial inner product in B . As $|b_J\rangle$ is chosen with quantum probability

$$\mathbb{P}(J = j) = \|\langle b_j | \Psi \rangle_B\|^2, \quad (9.10)$$

(9.9) is a random element of $\mathbb{S}(\mathcal{H}^S)$. In standard quantum mechanics (9.9) can be understood as the collapsed wave function of S after an ideal quantum measurement of the basis b on B . We saw above in Section 3.3.2 that (9.9) has been introduced in BM to explain the collapse postulate as well as the Born rule in standard quantum mechanics.

The state of S can be given by ψ^S or by $\hat{\rho}^S$. We first consider the standard textbook equilibrium ensembles and discuss the role of the ψ^S regarding thermal equilibrium later.

9.2. Thermodynamic Ensembles

Let us discuss the thermodynamic ensembles and their important role in equilibrium thermodynamics (see, e.g., [216, 244, 11]). In this Section we will see how the ensemble machinery works. Let $\hat{H}$ be a Hamiltonian and $\mathcal{H}_{\text{mc}}$ the micro-canonical energy shell with $\dim \mathcal{H}_{\text{mc}} = D$.

The **micro-canonical ensemble** is defined as follows. Consider the micro-canonical energy interval $I_{\text{mc}} = [E - \Delta E, E]$ with $\Delta E > 0$. Then the micro-canonical density

matrix is given by

$$\hat{\rho}_{\text{mc}} = \frac{1}{D} \mathbb{1}_{[E-\Delta E, E]}(\hat{H}), \quad (9.11)$$

with characteristic function $\mathbb{1}_A(x)$. Here $\mathbb{1}_{[E-\Delta E, E]}(\hat{H})$ denotes the orthogonal projection $\hat{P}_{\text{mc}}$ onto $\mathcal{H}_{\text{mc}}$. Hence we can also write $\hat{\rho}_{\text{mc}} = \hat{P}_{\text{mc}}/D$.

The **canonical density matrix** is given by

$$\hat{\rho}_{\text{can}} = \frac{1}{Z_{\text{can}}} e^{-\beta \hat{H}}, \quad (9.12)$$

with the canonical partition function

$$Z_{\text{can}} = \text{tr } e^{-\beta \hat{H}} \quad (9.13)$$

with inverse temperature $\beta = (k_{\text{B}}T)^{-1}$.

The **grand-canonical density matrix** is given by

$$\hat{\rho}_{\text{gc}} = \frac{1}{Z_{\text{gc}}} e^{-\beta(\hat{H} - \mu \hat{N})} \quad (9.14)$$

with particle number operator $\hat{N}$ and the grand-canonical partition function

$$Z_{\text{gc}} = \text{tr } e^{-\beta(\hat{H} - \mu \hat{N})}, \quad (9.15)$$

where μ is the chemical potential.

Relation to Thermodynamics

These three ensembles are related to three thermodynamic representations [121]. The micro-canonical ensemble is related to the entropy representation, the canonical ensemble is related to the free energy representation and the grand-canonical ensemble is related to the pressure representation.

In thermodynamics equilibrium properties can be determined by the entropy S , which is a function of extensive variables (see, e.g., [146, Ch. 6.3]); here we follow [121]. For a system with energy E , particle number N and volume V this reads

$$S = S(E, V, N). \quad (9.16)$$

There is a direct relation to other (intensive) variables via the derivatives of (9.16)

$$\frac{\partial S}{\partial E} = \frac{1}{T}, \quad \frac{\partial S}{\partial V} = -\frac{p}{T}, \quad \frac{\partial S}{\partial N} = -\frac{\mu}{T}, \quad (9.17)$$

with temperature T , pressure p and chemical potential μ ; as usual the variables to which one does not take the derivative are held fixed. Note that if (9.16) can be solved for E , such that $E = E(S, V, N)$ one obtains simpler derivatives.

There are other functional expressions in terms of intensive or extensive variables than (9.16). This can be done by Legendre transformation. For instance the free energy $F = F(T, V, N)$ is obtained from $E = E(S, V, N)$ via a Legendre transformation with respect to S and thus

$$F(T, V, N) = E - TS \quad (9.18)$$

with $T = \partial E / \partial S$. Further we have

$$\frac{\partial F}{\partial T} = -S, \quad \frac{\partial F}{\partial V} = -p, \quad \frac{\partial F}{\partial N} = \mu. \quad (9.19)$$

The grand-canonical representation is given thorough a Legendre transformation of $E = E(S, V, N)$ with respect to N and S and thus

$$\mathcal{G}(T, V, \mu) = E - TS - \mu N \quad (9.20)$$

with $\mu = \partial E / \partial N$. Further

$$\frac{\partial \mathcal{G}}{\partial T} = -S \quad \frac{\partial \mathcal{G}}{\partial V} = -p \quad \frac{\partial \mathcal{G}}{\partial \mu} = -N. \quad (9.21)$$

Other considerations can be made to obtain several thermodynamic potentials, which allow to compute relevant thermodynamic quantities, such as for instance specific heats.

To all these just mentioned thermodynamic potentials: (9.16) (9.18) (9.20), there is a corresponding ensemble. We will discuss this now. Thus there is an underlying microscopic description.

Microscopically the thermodynamic entropy is given by

$$S(E, V, N) = k_B \log Z_{\text{mc}} \quad (9.22)$$

where

$$Z_{\text{mc}} = \text{tr} \mathbf{1}_{[E-\Delta E, E]}(\hat{H}). \quad (9.23)$$

The free energy is expressed as follows

$$F(T, V, N) = -k_B T \log Z_{\text{can}} \quad (9.24)$$

with

$$\frac{\partial F}{\partial T} = -S_G, \quad (9.25)$$

further

$$\frac{\partial \log Z_{\text{can}}}{\partial \beta} = -\langle \hat{H} \rangle_{\text{can}} = \text{tr}(\hat{\rho}_{\text{can}} \hat{H}) \quad (9.26)$$

and

$$\frac{\partial \log Z_{\text{gc}}}{\partial \mu} = \beta \langle \hat{N} \rangle_{\text{gc}} = \beta \text{tr}(\hat{\rho}_{\text{gc}} \hat{N}). \quad (9.27)$$

Using the Gibbs entropy, the free energy reads

$$F(T, V, N) = \langle H \rangle_{\text{can}} + S_{\text{G}}(\hat{\rho}_{\text{can}}). \quad (9.28)$$

Finally, the pressure representation is given by the grand potential

$$\mathcal{G}(T, V, \mu) = -k_{\text{B}} T \log Z_{\text{gc}}. \quad (9.29)$$

Expectation values of common macro variables are given for instance by

$$\frac{\partial \mathcal{G}}{\partial \mu} = -\langle \hat{N} \rangle_{\text{gc}} = -\text{tr}(\hat{\rho}_{\text{gc}} \hat{N}). \quad (9.30)$$

That is as in TD formalism. Note that equilibrium properties can be computed without knowing anything about the dynamics.

It turns out that under certain conditions each of the just mentioned ensembles yield equivalent descriptions of macroscopic systems, known as **equivalence of ensembles**. Thus one can be pragmatic and choose the one that fits best for a certain problem. This has its roots in the relation of fundamental thermodynamic quantities through Legendre transformations [39]. Still there are some subtleties, where one has to be careful [75]. There are also cases where equivalence of ensembles actually fails [41].

The expressions above are exact. Note that one can also makes sense of ensembles as described here from the individualistic point of view as pointed out by Goldstein [121].

Derivation of Canonical Ensemble

Commonly the canonical and grand-canonical ensemble are derived from the micro-canonical ensemble. Let $\mathcal{H}_{\text{mc}}$ be the microcanonical energy shell with $\dim \mathcal{H}_{\text{mc}} = D$, which is a subspace of $\mathcal{H}^S \otimes \mathcal{H}^B$. We assume that S and B are weakly interacting and thus the Hamiltonian of $S \cup B$ is approximately given by $\hat{H} \approx \hat{H}^S + \hat{H}^B$. As an eigenbasis of $\mathcal{H}^S$, we choose an eigenbasis of $\hat{H}^S$ and as an eigenbasis of $\mathcal{H}^B$, we choose an eigenbasis of $\hat{H}^B$. It is assumed that $\hat{H}^S, \hat{H}^B$ have pure point spectrum and are bounded from below. Denote the eigenvalues of $\hat{H}^S$ as $E_1^S \leq E_2^S \leq \dots$ and the corresponding eigenvectors as $\phi_1^S, \phi_2^S, \dots$. Let the eigenvalues of $\hat{H}^B$ as $E_1^B \leq E_2^B \leq \dots$ and $\phi_1^B, \phi_2^B, \dots$ as the corresponding eigenvectors.

The reduced density matrix reads

$$\hat{\rho}^S = \text{tr}^B \hat{\rho}_{\text{mc}} = \frac{1}{D} \sum_i \dim(\mathcal{H}_i^B) |\phi_i^S\rangle \langle \phi_i^S| \quad (9.31)$$

with

$$\mathcal{H}_i^B = \mathcal{H}_{[E-E_i^S-\Delta E, E-E_i^S]}^B. \quad (9.32)$$

Its dimension can be computed for the entropy of the bath B , which for sufficiently large B , given by

$$S(E) \approx k_B \log \dim \mathcal{H}_{[E-\Delta E, E]}^{(B)} \quad (9.33)$$

such that by an expansion of 9.33

$$\dim \mathcal{H}_i^B \approx e^{S(E)} e^{-\beta E_i^S} \quad (9.34)$$

with the inverse temperature $\beta = 1/k_B T$. That is finally, the reduced density matrix $\hat{\rho}^S$ is indeed given by the canonical density matrix (9.12) with $\hat{H} = \hat{H}^S$. The grand-canonical density matrix can be derived in a similar vein with $\hat{H} = \hat{H}^S$ and $\hat{N} = \hat{N}^S$ the respective particle number operator on $\mathcal{H}^S$.

Generalized Gibbs Ensemble

Regarding the grand-canonical ensemble not only spatial equilibrium is of interest, but also chemical equilibrium. That is particle numbers do not only change, because particles move from some region to another (“spatial equilibrium”), but also due to chemical reactions of particle species A , B and C , such as



Here δE is the amount of energy consumed or released during the reaction. While spatial equilibrium is discussed in textbooks (see, e.g., [164, 244, 281]), chemical equilibrium is usually not (see for instance [188] for a nice treatment).

For chemical reactions the particle numbers of A , B and C are clearly not conserved, but during each reaction a linear combination of them is. Consider for instance the direction $A + B \rightarrow C + \delta E$. Now A goes down by one and B goes down by one, while C goes up by one. This means that $\hat{N}_A - \hat{N}_B$ is a conserved quantity during the reaction. A similar consideration for the reverse direction yields $\hat{N}_A + \hat{N}_C$ as a conserved quantity.

In a more general setting one can for suitable macroscopic variables define the

generalized Gibbs ensemble (see e.g. [11, 229, 164, 202])

$$\hat{\rho}_{\text{gG}} = \frac{1}{Z_{\text{gG}}} \exp \left(\sum_{k=1}^K \lambda_k \hat{Q}_k \right) \quad (9.36)$$

where Z_{gG} is the generalized partition function. The density matrix $\hat{\rho}_{\text{gG}}$ represents thermal equilibrium for those macroscopic variables $\hat{Q}_1, \dots, \hat{Q}_K$ that are conserved. We assume that these commute with each other. It follows that there is a K -parameter family of thermal equilibrium states with parameters $\lambda_1, \dots, \lambda_K$. As an example the canonical density matrix arises for $K = 1$ and $\hat{Q}_1 = \hat{H}$. Notice that the grand-canonical density matrix is more subtle as it does not only arise by setting $K = 2$ with $\hat{Q}_1 = \hat{H}$ and $\hat{Q}_2 = \hat{N}$.

Since energy is not the only conserved quantity anymore, we replace the micro-canonical subspace $\mathcal{H}_{\text{mc}}$ by the generalized micro-canonical subspace $\mathcal{H}_{\text{gmc}}$. The eigenvalues of each $\hat{Q}_k$ are pinned to an interval $[Q_k - \Delta Q_k, Q_k]$, short on the macroscopic length scale, but still large enough to contain many eigenvalues, i.e., $d_{\text{gmc}} = \dim \mathcal{H}_{\text{gmc}} \gg 1$, where

$$\mathcal{H}_{\text{gmc}} := \text{span} \left\{ \phi \in \mathcal{H} : \forall k : \hat{Q}_k \phi = q_k \phi, q_k \in [Q_k - \Delta Q_k, Q_k] \right\} \quad (9.37)$$

There is also a general version of the micro-canonical ensemble, the normalized projection

$$\hat{\rho}_{\text{gmc}} = \frac{\hat{P}_{\text{gmc}}}{d_{\text{gmc}}} \quad (9.38)$$

with $\hat{P}_{\text{gmc}}$ the projection onto (9.37).

Also in the generalized Gibbs ensemble equivalence of ensembles appears in two ways. First, it plays a role in the

General Gibbs Principle: Let $\hat{Q}_1, \dots, \hat{Q}_K$ be a collection of self-adjoint operators, that commute with each other, and large d_{gmc} . Then, in the relevant sense of equivalence of ensembles, $\hat{\rho}_{\text{gmc}}$ is equivalent to $\hat{\rho}_{\text{gG}}$ with λ_k chosen such that

$$\text{tr}(\hat{\rho}_{\text{gG}} \hat{Q}_k) = Q_k. \quad (9.39)$$

Second, that for a system $S \cup B$, two density matrices $\hat{\rho}_1$ and $\hat{\rho}_2$ are called S -equivalent if and only if

$$\text{tr}^B \hat{\rho}_1 \approx \text{tr}^B \hat{\rho}_2, \quad (9.40)$$

in trace norm⁵², that is

$$\|\mathrm{tr}^B \hat{\rho}_1 - \mathrm{tr}^B \hat{\rho}_2\|_{\mathrm{tr}} < \varepsilon \quad (9.41)$$

for sufficiently small $\varepsilon > 0$. Further $\hat{\rho}_1$ and $\hat{\rho}_2$ are locally equivalent if and only if for sufficiently small region S' , they are S' -equivalent. In [148] it is conjectured that besides exceptional choices of $\hat{Q}_k$,

$$\hat{\rho}_{\mathrm{gG}} \text{ locally equivalent to } \hat{\rho}_{\mathrm{gmc}}. \quad (9.42)$$

The general Gibbs ensembles are recently used in quantum statistical mechanics; see for instance [116, p. 19], [202] and the cited references therein. In particular the work by Rigol et al. [228], where the name “generalized Gibbs ensemble” was (to the knowledge of the author) introduced for the first time. Their motivation was to theoretically elaborate on an experiment, where the evolution towards a stationary state not equivalent to thermal equilibrium was observed (the reason is that conserved quantities “forbid” to reach thermal equilibrium; for more details see [228]). To describe this situation they refer to Jaynes [152], following the maximum entropy principle, that is maximizing von Neumann entropy

$$S_{\mathrm{vN}}(\hat{\rho}) = -k_{\mathrm{B}} \mathrm{tr} \hat{\rho} \log \hat{\rho} \quad (9.43)$$

with constraints given by the integrals of motion obtaining (9.36) and further fixing Lagrange multipliers λ_k by the initial condition

$$\mathrm{tr}(\hat{Q}_k \hat{\rho}) = \langle \hat{Q}_k \rangle(t=0). \quad (9.44)$$

The generalized Gibbs ensemble (9.36) turns out to be a useful tool to study equilibrium situations in statistical physics [11, Ch. 4]. For $\mathcal{H}_{\mathrm{gmc}}$ and constants of motion $\hat{Q}_k$ with $k \in [K]$ the average values

$$\langle \hat{Q}_k \rangle = \mathrm{tr}(\hat{\rho}_{\mathrm{gG}} \hat{Q}_k) \quad (9.45)$$

characterize equilibrium on the macroscopic level; to each of them one assigns a Lagrange multiplier λ_k . As above stated this yields a K -parameter family of thermal equilibrium states. A key role plays the normalization constant Z_{gG} in (9.36). The averages of (9.45) can also be computed via

$$\langle \hat{Q}_k \rangle = -\frac{\partial}{\partial \lambda_k} \log Z_{\mathrm{gG}} \quad (9.46)$$

⁵²Let $\hat{A}$ be a self-adjoint operator on $\mathcal{H}$, then the trace norm is given by $\|\hat{A}\|_{\mathrm{tr}} = \mathrm{tr} \sqrt{\hat{A}^* \hat{A}}$, where $\hat{A}^*$ denotes the adjoint of $\hat{A}$.

where

$$Z_{\text{gG}} = \text{tr} \exp \left(\sum_{k=1}^K \lambda_k \hat{Q}_k \right). \quad (9.47)$$

In equilibrium the **generalized Gibbs entropy** using (9.45) is given by

$$S_{\text{gG}}(\hat{\rho}_{\text{gG}}) = k_{\text{B}} \log Z_{\text{gG}} - k_{\text{B}} \sum_{k=1}^K \lambda_k \frac{\partial}{\partial \lambda_k} \log Z_{\text{gG}}. \quad (9.48)$$

Further thermodynamic expressions can be obtained from there; for example for $K = 1$ with $\hat{Q}_1 = \hat{H}$, this boils down to (9.28).

9.3. Microscopic Thermal Equilibrium (MITE)

Above in Section 2.4 we introduced MATE. For smaller systems, such as subsystems S contained in an environment a similar notion, commonly used (see e.g. [180, 218, 204, 230]), exists: microscopic thermal equilibrium (MITE). It is “more” microscopic than MATE, which means that it takes the locality of certain observables into account, as these are defined on microscopic length scales. Its conceptual relevance was first worked out by [127, 128] and it is defined as follows: a system S is in MITE if its wave function $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ with $\mathcal{H}_{\text{mc}} \subset \mathcal{H}^S \otimes \mathcal{H}^B$ is such that

$$\hat{\rho}_{\psi}^S \approx \hat{\rho}_{\text{mc}}^S \quad (9.49)$$

where $\hat{\rho}_{\psi}^S = \text{tr}^{\bar{S}} |\psi\rangle\langle\psi|$. More precisely for any subsystem $S \subset \Lambda$, let $\text{diam}(S)$ be its diameter. Then MITE_{ℓ} (“MITE at length scale ℓ ”) reads

$$\text{MITE}_{\ell} = \bigcap_{S: \text{diam}(S) \leq \ell} \{ \psi \in \mathbb{S}(\mathcal{H}_{\text{mc}}) : \hat{\rho}_S^{\psi} \approx \hat{\rho}_S^{\text{mc}} \}. \quad (9.50)$$

Then MITE is defined through MITE_{ℓ_0} for specific ℓ_0 : let ℓ_0 be the largest ℓ , but still small enough, to make sure that for each S with $\text{diam}(S) \leq \ell_0$: $\hat{\rho}_{\text{mc}}^S \approx \hat{\rho}_{\text{can}}^S$.

MITE has some interesting properties [127, 128]. Clearly, any state $\psi \in \text{MITE}_{\ell}$ is also in $\text{MITE}_{\ell'}$ for $0 < \ell' < \ell$. As a consequence one can extend MITE to a collection of regions $S_i \subset \Lambda$, allowing to make statements about how large S can be. Further most $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ lie in MITE (for a precise statement see Section 11.1).

MITE is a purely quantum notion having its roots in entanglement as a pure state of $S \cup B$ can lead to a mixed state of S (think of two entangled spin-1/2 particles). For a classical system MITE does not exist. Given a phase point (the analog of a pure state in classical mechanics) X of $S \cup B$, tracing out the degrees of freedom of B yields again a phase point X_S (and not a probability distribution, which would be

the classical analog of a mixed state); for more details see [127, 128].

MITE and MATE are not equivalent, as MITE implies MATE but not the other way around. Still they are part of a general scheme. Let us explain.

MITE implying MATE can be seen like this. Let $\hat{A}$ be a self-adjoint operator, then the probability distribution defined on the spectrum of $\hat{A}$ is for $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ given by

$$\mathbb{P}_A^\psi(B) = \langle \psi | \hat{P}_A(B) | \psi \rangle \quad (9.51)$$

for any $B \subseteq \mathbb{R}$. Here $\hat{P}_A(B)$ denotes the PVM on the real line given by spectral decomposition of $\hat{A}$. In the same vein there's a probability distribution given through the micro-canonical ensemble

$$\mathbb{P}_A^{\text{mc}}(B) = \text{tr}(\hat{P}_A(B) \hat{\rho}_{\text{mc}}) \quad (9.52)$$

also with $B \subseteq \mathbb{R}$.

Note that for $\hat{A} = \hat{A}^S \otimes \hat{I}^{\bar{S}}$ and $\psi \in \text{MITE}_\ell$

$$\mathbb{P}_A^{\text{mc}}(B) = \text{tr}(\hat{P}_A(B) \hat{\rho}_{\text{mc}}) = \text{tr}(\hat{P}_{\hat{A}^S}(B) \hat{\rho}_{\text{mc}}^S) \approx \text{tr}(\hat{P}_{\hat{A}^S}(B) \hat{\rho}_\psi^S) = \mathbb{P}_A^\psi(B) \quad (9.53)$$

for arbitrary $B \subseteq \mathbb{R}$. Given this it is easy to see that MATE follows from MITE. Let L be the length scale of certain macroscopic observables. Then suppose that for $L \leq \ell_0$ the system is in MITE, i.e., $\hat{\rho}_\psi^S \approx \hat{\rho}_{\text{mc}}^S$ holds at least up to L . Choosing appropriate values of L (say $10^{-4}m$) and ℓ_0 (say $10^{-3}m$) this is certainly the case. Hence the upshot is: if $\psi \in \text{MITE}$, then $\psi \in \text{MATE}$.

MATE and MITE are part of a more general scheme in the following sense: think of a set of observables $\mathcal{A}$. Then a system is in thermal equilibrium relative to $\mathcal{A}$ if its state ψ satisfies that for each observable $\hat{A} \in \mathcal{A}$, one has

$$\langle \psi | \hat{A} | \psi \rangle \approx \text{tr}(\hat{A} \hat{\rho}_{\text{mc}}). \quad (9.54)$$

In particular this means that for observables of the form $\hat{A} = \sum_\alpha \alpha \hat{P}_\alpha$ the probability distribution

$$p(\alpha) = \langle \psi | \hat{P}_\alpha | \psi \rangle \quad (9.55)$$

is approximated by that of the micro-canonical ensemble $\hat{\rho}_{\text{mc}}$, i.e.,

$$\langle \psi | \hat{P}_\alpha | \psi \rangle \approx \text{tr}(\hat{\rho}_{\text{mc}} \cdot \hat{P}_\alpha) \quad (9.56)$$

One obtains MATE for $\mathcal{A} = \mathcal{A}_{\text{MATE}}$ and MITE for $\mathcal{A} = \mathcal{A}_{\text{MITE}}$, where $\mathcal{A}_{\text{MATE}} = \{\hat{M}_1, \dots, \hat{M}_K\}$ and $\mathcal{A}_{\text{MITE}}$ consists of the collection of subsets

$$\mathcal{A}_S = \{\hat{A}_0 \otimes \hat{I}^{\bar{S}} : \hat{A}_0 \text{ self-adjoint on } \mathcal{H}^S\}, \quad (9.57)$$

that is $\mathcal{A}_{\text{MITE}} = \cup_S \mathcal{A}_S$ (where the union is taken over all spatial regions S with diameter less or equal to ℓ_0).

MATE does not imply MITE, which means that from $\langle \psi | \hat{P}_{\text{eq}} | \psi \rangle$ it does not follow that $\hat{\rho}_\psi^S \approx \hat{\rho}_{\text{mc}}^S$. In a nutshell MATE does not account for the microscopic aspects, and thus there can be wave functions which do not lie in MITE (for more details see [127, 128]).

9.4. Approach to MITE

Let us now discuss the approach to MITE. As for the approach to MATE, the central condition for the approach to MITE is the MITE-ETH, which states that the eigenstates of $\hat{H}$ lie in MITE.

Approaches [228, 218, 180, 219] relying on the MITE-ETH also assuming that $\hat{H}$ has non-degenerate energy gaps (“no resonances”)

$$E_n - E_m \neq E_{n'} - E_{m'} \quad (9.58)$$

unless either $n = n'$ and $m = m'$ or $n = m$ and $n' = m'$, a condition fulfilled for generic Hamiltonians [279, Appendix A].

There are different statements showing the approach to MITE using the MITE-ETH, which either show that *most* initial states [218, 180] or *any* initial state [259, 260] reaches MITE and stays there for most of the time (in the long run). We focus on the latter for now and discuss the other statements below.

More explicitly, let ϕ_n, ϕ_m be eigenvectors of $\hat{H}$ with different eigenvalues, then the MITE-ETH says that $\langle \phi_n | \hat{A} | \phi_n \rangle \approx \text{tr}(\hat{A} \hat{\rho}_{\text{mc}})$ (diagonal ETH) and $\langle \phi_n | \hat{A} | \phi_m \rangle \approx 0$ (off-diagonal ETH). If that is the case, then any initial state will reach MITE and stays there for most of the time (in the long run) [259, 260].

This can be seen as follows: let $\hat{A} \in \mathcal{A}_{\text{MITE}}$ and let $\psi_0 \in \mathbb{S}(\mathcal{H}_{\text{mc}})$, where $\mathcal{H}_{\text{mc}} \subseteq \mathcal{H}^S \otimes \mathcal{H}^B$, such that

$$|\psi_0\rangle = \sum_n c_n |\phi_n\rangle \quad \text{and} \quad |\psi_t\rangle = \sum_n e^{-itE_n} c_n |\phi_n\rangle, \quad (9.59)$$

where $c_n = \langle \phi_n | \psi_0 \rangle$. Now the aim is to get a stationary state, which is done by computing the time average

$$\overline{\langle \psi_t | \hat{A} | \psi_t \rangle} = \sum_{n,m} \overline{e^{-it(E_m - E_n)}} c_n^* c_m \langle \phi_n | \hat{A} | \phi_m \rangle \quad (9.60)$$

$$= \sum_n |c_n|^2 \langle \phi_n | \hat{A} | \phi_n \rangle \quad (9.61)$$

$$\approx \text{tr}(\hat{\rho}_{\text{mc}} \hat{A}). \quad (9.62)$$

9. Thermal Equilibrium of Subsystems

Here the last line follows by the diagonal ETH of Srednicki from above. In order to show that this holds for most times, one has to show that the time variance is small. This is quite tedious, but straightforward; the upshot is that

$$\overline{\left(\langle\psi_t|\hat{A}|\psi_t\rangle - \overline{\langle\psi_t|\hat{A}|\psi_t\rangle}\right)^2} = \sum_{n \neq m} |c_n|^2 |c_m|^2 |\langle\phi_n|\hat{A}|\phi_m\rangle|^2 \approx 0, \quad (9.63)$$

which follows from the off-diagonal ETH of Srednicki above. Hence the MITE-ETH provides that for any initial state and all $\hat{A} \in \mathcal{A}_{\text{MITE}}$

$$\langle\psi_t|\hat{A}|\psi_t\rangle \approx \text{tr}(\hat{\rho}_{\text{mc}}\hat{A}) \quad (9.64)$$

for most times in the long run. Stated differently from a more individualistic perspective it means that $\psi_t \in \text{MITE}$ for most times in the long run.

This can be made mathematically precise and looks as follows [284]: let $\delta, \eta > 0$ and let $\hat{H}$ be a non-degenerate Hamiltonian with non-degenerate energy gaps and let $\hat{A} \in \mathcal{A}_{\text{MITE}}$. With $\varepsilon = \sqrt{\eta}\delta/2$ we assume that

$$\forall n \forall \hat{A} : \quad |\langle\phi_n|\hat{A}|\phi_n\rangle - \text{tr}(\hat{A}\hat{\rho}_{\text{mc}})| < \varepsilon \quad (9.65)$$

and

$$\forall n \neq m \forall \hat{A} : \quad |\langle\phi_n|\hat{A}|\phi_m\rangle| < \varepsilon. \quad (9.66)$$

Then, for any $\psi_0 \in \mathbb{S}(\mathcal{H}_{\text{mc}})$, every $\hat{A}$, for $(1 - \eta)$ -most t

$$|\langle\psi_t|\hat{A}|\psi_t\rangle - \text{tr}(\hat{A}\hat{\rho}_{\text{mc}})| < \delta. \quad (9.67)$$

To show that this is the case is, as mentioned, straightforward but quite tedious, so we do not state it here (see [284, 128]).

A similar statement is true for Hamiltonians $\hat{H}$ with degenerate energy gaps, where the proof shares some similarities. We now discuss how initial states $\psi_0 \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ reach MITE and stay there for most of the time (in the long run) [148]:

Let $\varepsilon, \delta > 0$, $\mathcal{H} = \mathcal{H}^S \otimes \mathcal{H}^B$, let $\mathcal{H}_R \subset \mathcal{H}$ be a subspace, $\hat{P}_R$ the projection to $\mathcal{H}_R$, and $\hat{H}$ a Hamiltonian on $\mathcal{H}$ such that $[\hat{H}, \hat{P}_R] = 0$. Moreover, suppose (MITE-ETH) that for any eigenvectors $\phi_1, \phi_2 \in \mathbb{S}(\mathcal{H}_R)$ of $\hat{H}$ with eigenvalues $E_1 \neq E_2$,

$$\left\| \text{tr}^B |\phi_1\rangle\langle\phi_1| - \text{tr}^B \hat{\rho}_R \right\|_2 < \varepsilon, \quad (9.68)$$

$$\left\| \text{tr}^B |\phi_1\rangle\langle\phi_2| \right\|_2 < \varepsilon, \quad (9.69)$$

where $\|\cdot\|_2$ denotes the Hilbert-Schmidt norm. Then every $\psi_0 \in \mathbb{S}(\mathcal{H}_R)$ is such that

for $(1 - \delta)$ -most $t \in [0, \infty)$,

$$\left\| \text{tr}^B |\psi_t\rangle\langle\psi_t| - \text{tr}^B \hat{\rho}_R \right\|_2 < 2\varepsilon \sqrt{\frac{D_G}{\delta}}, \quad (9.70)$$

where D_G is the maximal degeneracy of eigenvalue gaps,

$$D_G := \max_{\tilde{E} \in \mathbb{R}} \# \{ (E, E') \in \mathcal{E} \times \mathcal{E} : E \neq E' \text{ and } E - E' = \tilde{E} \}, \quad (9.71)$$

and $\mathcal{E}$ the set of eigenvalues of $\hat{H}$.

Given the MITE-ETH, thermalization follows quite trivially. The hard part is to show that the MITE-ETH actually holds. This has not been done in full generality yet. Investigating the ETH is a vast research field of its own (see, e.g., [202, 116, 74, 31] and references therein).

Nevertheless we want to discuss some results here. These are related to random Hamiltonians, that is the MITE-ETH does not hold for all energy eigenstates, but for most of them. Results that have shown the typicality of the MITE-ETH are for instance [221, 202].

Note further that there are systems that are not in MITE. This can be seen as follows: think of $\hat{H}$ that has eigenvectors either lying in $\mathcal{H}_{\text{eq}}$ or not and thus being orthogonal to it [9]. That is not only a mathematically constructed example, but also appears in real systems. Such systems are known to obey many body localization (MBL) or Anderson localization [127, 128]. There, energy eigenstates are localized in space, such that they can never get to thermal equilibrium. For other systems obeying a violation of the MITE-ETH see [202, 116] and the cited references therein.

10. Thermal Distribution of Wave Functions

We will now discuss how the conditional wave function $\psi^S \in \mathbb{S}(\mathcal{H}^S)$ is distributed in thermal equilibrium. To do so, we need to assign a measure to the set of such wave functions. Afterwards we state the properties of this measure and argue why it serves as a probability distribution for wave functions in thermal equilibrium. It turns out that these are the typical measures. This investigation has first been done in the seminal work of Goldstein et al. [134] and followed further in [218, 132] and also recently in [296, 279, 148, 290]. These results show that wave functions can also describe the thermal behavior of a subsystem properly and thus support the individualistic view; in this section we mostly follow [134, 132, 284].

To get an idea of these measures let us consider classical statistical mechanics first. Here, thermal equilibrium distributions of a subsystem S are represented by the corresponding canonical ensembles. These refer to probability distributions over phase space. Consider for instance the canonical ensemble with probability density $\rho_{\text{can}} = Z^{-1} \exp(-\beta H_S)$, where H_S is the Hamilton function of S , and corresponding canonical measure μ_{can} . That means in thermal equilibrium a phase point $X \in \Gamma^S$ has as its distribution μ_{can} , i.e.,

$$X \sim \mu_{\text{can}}. \quad (10.1)$$

The question that arises now is: can this also be done in the quantum realm? Is there a measure μ_{eq} on $\mathbb{S}(\mathcal{H}^S)$, such that for a wave function $\psi^S \in \mathbb{S}(\mathcal{H}^S)$, in thermal equilibrium,

$$\psi^S \sim \mu_{\text{eq}}. \quad (10.2)$$

It turns out that there is such a measure μ_{eq} , called GAP measure, which we will discuss below and show how it is related to thermal equilibrium. That question is particularly interesting in quantum mechanics as it is related directly to density matrices, which arise as statistical operators. For $\Psi \in \mathbb{S}(\mathcal{H})$ with $\Psi \sim \mu$, where μ is a measure μ on $\mathbb{S}(\mathcal{H})$, one can assign a density matrix to μ as a statistical operator (“statistical mixture”)

$$\hat{\rho}_\mu = \int_{\mathbb{S}(\mathcal{H})} \mu(d\psi) |\psi\rangle\langle\psi|, \quad (10.3)$$

which is equivalent to

$$\hat{\rho}_\mu = \mathbb{E}|\Psi\rangle\langle\Psi|, \quad (10.4)$$

where $\mathbb{E}$ is the expectation value with respect to μ . It is well known that density matrices are used to compute statistics of measurement outcomes. As discussed in Section 9.1 two different measures $\mu_1 \neq \mu_2$ on $\mathbb{S}(\mathcal{H})$ can yield the same density matrix. We will now show that for each $\hat{\rho}$ on $\mathcal{H}$, there is a unique measure $\text{GAP}_{\hat{\rho}}$ called the GAP measure. GAP is an acronym and stands for Gaussian, adjusted and projected measure. It is the most spread out distribution over $\mathbb{S}(\mathcal{H})$ with density matrix $\hat{\rho}$, in such a way that $\hat{\rho}_{\text{GAP}_{\hat{\rho}}} = \hat{\rho}$, also known was the ‘‘Scrooge’’ measure [156]. Recent considerations involving such measures has also been done in [201, 192, 196].

We proceed as follows: in Section 10.1 we define the GAP measure and in Section 10.2 its properties. Afterwards in Section 10.3 we show how the GAP measure used as the distribution of a wave function in thermal equilibrium. We end in Section 10.4 with the relation of GAP measures and normal typicality.

10.1. GAP Measure

We now discuss how the GAP measure is build up; notice that there are at least four ways to define the GAP measure [132, Sec. 2]; here we follow [134].

Let $\hat{\rho}$ be a density matrix on a Hilbert space $\mathcal{H}$ with $\dim \mathcal{H} = D$. Let $G_{\hat{\rho}}$ be the Gaussian measure on $\mathcal{H}$ with mean zero and covariance matrix $\hat{\rho}$. More precisely, consider the spectral decomposition

$$\hat{\rho} = \sum_n p_n |n\rangle\langle n|, \quad (10.5)$$

where $\{|n\rangle\}$ is an eigenbasis of $\hat{\rho}$ and the p_n are the eigenvalues of $\hat{\rho}$.

Now consider independent complex valued Gaussian random variables $(Z_1, \dots, Z_D)$, more precisely $Z_n \sim \mathcal{N}_{\mathbb{C}}(0, p_n)$ for $n \in [D]$ and note that

$$\sum_n p_n |n\rangle\langle n| = \sum_n \mathbb{E}|Z_n|^2 |n\rangle\langle n|. \quad (10.6)$$

One defines the distribution $G_{\hat{\rho}}$ as the distribution of the random vector $\Psi^G = \sum_n Z_n |n\rangle \sim G_{\hat{\rho}}$. We have that $\mathbb{E}\Psi^G = 0$ and

$$\mathbb{E}||\Psi^G||^2 = \sum_n \mathbb{E}|Z_n|^2 = \sum_n p_n = \text{tr } \hat{\rho} = 1. \quad (10.7)$$

It is even more generally the case that for an arbitrary measure μ on $\mathcal{H}$, which has

mean zero and covariance C given by

$$C = \int_{\mathcal{H}} \mu(d\psi) |\psi\rangle\langle\psi|, \quad (10.8)$$

a random vector $\Psi \sim \mu$ has $\mathbb{E}||\Psi||^2 = \text{tr } C$.

We need a measure on $\mathbb{S}(\mathcal{H})$ and not on $\mathcal{H}$. One would expect to project $G_{\hat{\rho}}$ onto $\mathbb{S}(\mathcal{H})$. As the covariance changes by doing that, this is not possible. However there's a way to circumvent this problem. Introduce an adjustment factor, which takes care of that. The adjusted Gaussian measure $\text{GA}_{\hat{\rho}}$ on $\mathcal{H}$ is defined as

$$\text{GA}_{\hat{\rho}}(d\psi) = ||\psi||^2 G_{\hat{\rho}}(d\psi). \quad (10.9)$$

By (10.7) this is indeed a probability measure. Now let $\Psi^{\text{GA}} \sim \text{GA}_{\hat{\rho}}$ and then

$$\Psi^{\text{GAP}} = \frac{\Psi^{\text{GA}}}{||\Psi^{\text{GA}}||} = P(\Psi^{\text{GA}}). \quad (10.10)$$

Here we used that the mapping $P : \mathcal{H} \setminus \{0\} \rightarrow \mathbb{S}(\mathcal{H})$ where $P(\psi) = ||\psi||^{-1}\psi$ and thus $\Psi^{\text{GAP}} = P(\Psi^{\text{GA}})$. The upshot is that

$$\Psi^{\text{GAP}} \sim \text{GAP}_{\hat{\rho}}. \quad (10.11)$$

So far the GAP measure has been ascribed more abstractly as the distribution of the vector Ψ^{GAP} . A more explicit look at the GAP measure is as follows. First let $B \subseteq \mathbb{S}(\mathcal{H})$, then

$$\text{GAP}_{\hat{\rho}}(B) = \text{GA}_{\hat{\rho}}(\mathbb{R}^+ B) = \int_{\mathbb{R}^+ B} G_{\hat{\rho}}(d\psi) ||\psi||^2, \quad (10.12)$$

where the cone through B is written as $\mathbb{R}^+ B$. Second, for finite-dimensional $\mathcal{H}$, one can express $\text{GA}_{\hat{\rho}}$ and $\text{GAP}_{\hat{\rho}}$ in terms of their probability densities with respect to the uniform distribution u on $\mathbb{S}(\mathcal{H})$. Let λ denote the Lebesgue measure on $\mathbb{C}^D$, then

$$\frac{dG_{\hat{\rho}}}{d\lambda}(\psi) = \frac{1}{\pi^D \det \hat{\rho}} \exp(-\langle \psi | \hat{\rho}^{-1} | \psi \rangle) \quad (10.13)$$

$$\frac{d\text{GA}_{\hat{\rho}}}{d\lambda}(\psi) = \frac{||\psi||^2}{\pi^D \det \hat{\rho}} \exp(-\langle \psi | \hat{\rho}^{-1} | \psi \rangle) \quad (10.14)$$

$$\frac{d\text{GAP}_{\hat{\rho}}}{du}(\psi) = \frac{D!}{2\pi^D \det \hat{\rho}} \langle \psi | \hat{\rho}^{-1} | \psi \rangle^{-D-1}, \quad (10.15)$$

where we assumed that all eigenvalues of $\hat{\rho}$ are greater than zero. Note that comparing the densities one really sees that the covariance matrix is given by $\hat{\rho}$. For a

consideration that makes use of the densities more explicitly see [218].

10.2. Properties of the GAP Measure

We now state properties of the GAP measure. Some of them will be needed later on and some of them are just mentioned due to completeness.

First we need to introduce some notation. Let $\hat{\rho}$ be a density matrix on a finite-dimensional Hilbert space $\mathcal{H}$ with $\dim \mathcal{H} = D$. For $\gamma \in (0, 1/D)$ let $\mathcal{D}_{\geq \gamma}(\mathcal{H})$ denote the set of density matrices on $\mathcal{H}$ with eigenvalues greater or equal to γ . Further, for an arbitrary measure μ on $\mathbb{S}(\mathcal{H})$ and any measurable function $f : \mathbb{S}(\mathcal{H}) \rightarrow \mathbb{C}$ we define

$$\mu(f) := \int_{\mathbb{S}(\mathcal{H})} f(\psi) \mu(d\psi). \quad (10.16)$$

This will be needed in order to treat differences between measures below. This will be relevant to tell when a probability measure is close to the GAP measure. Further $\|M\|_{\text{tr}} = \text{tr} |M| = \text{tr} \sqrt{M^* M}$ denotes the trace norm. Now we collect some properties of GAP measures.

- (1) By construction $\hat{\rho} = \hat{\rho}_{\text{GAP}_{\hat{\rho}}}$, i.e., the GAP measure has covariance $\hat{\rho}$. This can be seen as follows

$$\hat{\rho}_{\text{GAP}_{\hat{\rho}}} = \int_{\mathbb{S}(\mathcal{H})} \text{GAP}_{\hat{\rho}}(d\psi) |\psi\rangle\langle\psi| \quad (10.17)$$

$$= \mathbb{E} (|\Psi^{\text{GAP}}\rangle\langle\Psi^{\text{GAP}}|) \quad (10.18)$$

$$= \int_{\mathcal{H}} \text{GA}_{\hat{\rho}}(d\psi) \|\psi\|^{-2} |\psi\rangle\langle\psi| \quad (10.19)$$

$$= \int_{\mathcal{H}} \text{G}_{\hat{\rho}}(d\psi) |\psi\rangle\langle\psi| = \hat{\rho}, \quad (10.20)$$

where the last equality follows from the fact that the covariance matrix of $\text{G}_{\hat{\rho}}$ is given by $\hat{\rho}$. The steps before mainly rely on the definitions of Ψ^{GAP} , $\text{GA}_{\hat{\rho}}$ etc. (see above).

- (2) Let U be a unitary operator on $\mathcal{H}$, then

$$U_* \text{GAP}_{\hat{\rho}} = \text{GAP}_{U \hat{\rho} U^\dagger}, \quad (10.21)$$

where $U^\dagger = U^{-1}$ and U_* is how U acts on measures, namely via $U_* \mu = \mu \circ U^{-1}$. An important consequence is that under unitary evolution $\text{GAP}_{\hat{\rho}}$ is stationary for the thermodynamic density matrices. That makes it a natural candidate for a typicality measure (see 11.1).

- (3) If $\Psi \in \mathcal{H}^S \otimes \mathcal{H}^B$ has $\text{GAP}_{\hat{\rho}^S \otimes \hat{\rho}^B}$ as its distribution, then for an arbitrary basis b of $\mathcal{H}^B$, one has $\Psi^S \sim \text{GAP}_{\hat{\rho}^S}$. This property of the GAP measure is called hereditary.
- (4) Let $\mathcal{H}_\nu \subset \mathcal{H}$ and $\hat{\rho}_\nu = \hat{P}_\nu/d_\nu$ with $\hat{P}_\nu$ projecting onto $\mathcal{H}_\nu$, then

$$\text{GAP}_{\hat{\rho}_\nu} = u_\nu. \quad (10.22)$$

Here u_ν denotes the uniform distribution on $\mathbb{S}(\mathcal{H}_\nu)$. A property that is particularly interesting for the micro-canonical density matrix $\hat{\rho}_{\text{mc}} = \hat{P}_{\text{mc}}/d$, where $\hat{P}_{\text{mc}}$ projects onto the micro-canonical energy shell $\mathcal{H}_{\text{mc}}$ and $\dim \mathcal{H}_{\text{mc}} = d$, as in this case $\text{GAP}_{\hat{\rho}_{\text{mc}}} = u_{\text{mc}}$. That is, the distribution of ψ^S is u_{mc} (analogously in classical mechanics for a phase point of a closed system in thermal equilibrium).

- (5) For $b \sim u_{\text{ONB}(\mathcal{H})}$ (recall the notion of a uniformly distributed ONB b from Section 2.3)

$$\mathbb{E} \mu_{\psi, b}^S = \text{GAP}_{\hat{\rho}_\psi^S}, \quad (10.23)$$

where $\mu_{\psi, b}^S(A) = \mathbb{P}(\psi^S \in A)$ with $A \subseteq \mathbb{S}(\mathcal{H}^S)$; see [132, p.973].

- (6) Continuity of GAP measures: for every $\varepsilon \in (0, 1)$, every $d \in \mathbb{N}$, there is a number $r = r(\varepsilon, d, f) > 0$ such that for all $\hat{\rho}, \hat{\Omega} \in \mathcal{D}(\mathcal{H})$,

$$\text{if } \|\hat{\rho} - \hat{\Omega}\|_{\text{tr}} < r, \text{ then } |\text{GAP}_{\hat{\rho}}(f) - \text{GAP}_{\hat{\Omega}}(f)| < \varepsilon. \quad (10.24)$$

- (7) Let ε, d be as in (6). Let $u_{\mathbb{S}(\mathcal{H})}$ denote the (normalized) uniform measure on $\mathbb{S}(\mathcal{H})$. Let $\hat{\rho} \in \mathcal{D}(\mathcal{H})$, $\text{GAP}_{\hat{\rho}}$ has a density relative to $u_{\mathbb{S}(\mathcal{H})}$, given that $\hat{\rho}$ has non-zero eigenvalues. Further for every $0 < \gamma < 1/d$, there is a number $r = r(\varepsilon, d, \gamma)$, such that for all $\hat{\rho}, \gamma \in \mathcal{D}_{\geq \gamma}(\mathcal{H})$,

$$\text{if } \|\hat{\rho} - \hat{\Omega}\|_{\text{tr}} < r, \text{ then } \left\| \frac{d\text{GAP}_{\hat{\rho}}}{du_{\mathbb{S}(\mathcal{H})}} - \frac{d\text{GAP}_{\hat{\Omega}}}{du_{\mathbb{S}(\mathcal{H})}} \right\|_{\infty} < \varepsilon. \quad (10.25)$$

What follows from this is that for such $\hat{\rho}, \hat{\Omega}$,

$$|\text{GAP}_{\hat{\rho}}(f) - \text{GAP}_{\hat{\Omega}}(f)| < \varepsilon \|f\|_1 \quad (10.26)$$

with f any element of $L^1(\mathbb{S}(\mathcal{H}), u_{\mathbb{S}(\mathcal{H})})$; here $\|\cdot\|_{\infty}$ denotes the sup-norm.

- (8) GAP measure for conditional wave function [279]: let $\varepsilon, \delta \in (0, 1)$ and let $\mathcal{H} = \mathcal{H}^S \otimes \mathcal{H}^B$ with $\mathcal{H}^S$, where $\dim \mathcal{H}^S = d_S$, and $\mathcal{H}^B$ be finite dimensional, such that $d_B \geq C(d_S, \varepsilon, \delta)$. Let $f : \mathbb{S}(\mathcal{H}^S) \rightarrow \mathbb{R}$ be an arbitrary continuous function. Then there exists a $p > 0$ in such a way that for any density matrix

$\hat{\rho}$ on $\mathcal{H}$ with $\|\hat{\rho}\| \leq p$,

$$\text{GAP}_{\hat{\rho}} \times u_{\text{ONB}} \left\{ (\psi, b) \in \mathbb{S}(\mathcal{H}) \times \text{ONB}(\mathcal{H}^B) : \right. \quad (10.27)$$

$$\left. |\mu_{\psi, b}^S(f) - \text{GAP}_{\text{tr}^B \hat{\rho}}(f)| < \varepsilon \right\} \geq 1 - \delta. \quad (10.28)$$

10.3. GAP Measure as Thermal Distribution

The motivation for the GAP measure has been to serve as the distribution of the conditional wave function in thermal equilibrium. We now get to this point by making use of some of the properties of GAP measures mentioned above.

To see that ψ^S has $\text{GAP}_{\hat{\rho}_{\text{can}}}$ as its thermal equilibrium distribution for a sufficiently large heat bath B we need the following theorem [132, Thm. 4].

Theorem 10.3.1. *Let $\varepsilon, \delta \in (0, 1)$, $d_S \in \mathbb{N}$ and $\gamma \in (0, 1/d_S)$. Then there are numbers $D_R = D_R(\varepsilon, \delta, d_S, \gamma) > 0$ and $r = r(\varepsilon, d_S, \gamma) > 0$, such that for every $d_R \in \mathbb{N}$ with $d_R > D_R$, for every $\mathcal{H}^S$, for every $\hat{\Omega} \in \mathcal{D}_{\geq \gamma}(\mathcal{H}^S)$, for every $\mathcal{H}^B$ and $\mathcal{H}_R \subseteq \mathcal{H}^S \otimes \mathcal{H}^B$ with $\dim \mathcal{H}_R = d_R$ satisfying*

$$\|\text{tr}^B \hat{\rho}^R - \hat{\Omega}\|_{\text{tr}} < r, \quad (10.29)$$

and for every bounded measurable function $f : \mathbb{S}(\mathcal{H}_R) \rightarrow \mathbb{C}$,

$$u_R \times u_{\text{ONB}} \left\{ (\psi, b) \in \mathbb{S}(\mathcal{H}_R) \times \text{ONB}(\mathcal{H}^B) : \right. \quad (10.30)$$

$$\left. |\mu_{\psi, b}^S(f) - \text{GAP}_{\hat{\Omega}}(f)| < \varepsilon \|f\|_{\infty} \right\} \geq 1 - \delta. \quad (10.31)$$

Note that this (loosely speaking) means the GAP-measure is the typical measure.

We now consider the canonical setup. Let $\mathcal{H} = \mathcal{H}^S \otimes \mathcal{H}^B$ and $\mathcal{H}_R = \mathcal{H}_{\text{mc}} \subseteq \mathcal{H}$. Further assume that S and B are weakly coupled, therefore

$$\hat{H} \approx \hat{H}^S \otimes \hat{I}^B + \hat{I}^S \otimes \hat{H}^B \quad (10.32)$$

with $\hat{H}^S$ and $\hat{H}^B$ the respective Hamiltonians on $\mathcal{H}^S$ and $\mathcal{H}^B$; further assume that the eigenvalues of $\hat{H}^B$ are sufficiently dense, which means that B has to be large enough. It is well known that

$$\text{tr}^B \hat{\rho}_{\text{mc}} \approx \frac{1}{Z_{\text{can}}} e^{-\beta H^S} \quad (10.33)$$

for suitable choice of $\beta = (k_B T)^{-1}$; here T is the temperature of B (compare (9.12)).

It follows from 10.3.1, that for most $\psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ and for most ONBs b of $\mathcal{H}^B$,

$$\mu_{\psi,b}^S \approx \text{GAP}_{\hat{\rho}_{\text{can}}}. \quad (10.34)$$

Remark 10.3.2. There is another way to see this using the hereditary property of the GAP measure (see Appendix 11.2 or [134, Sec.4]). $\diamond$

10.4. Generalized Normal Typicality

Normal typicality has been established for initial states distributed according to the uniform measure on the unit sphere. As we have seen above, this measure is a special instance of the GAP measure for a density matrix projecting onto a certain subspace and being normalized by the dimension of that subspace. Hence a natural question is, whether this can be extended to GAP measures.

The answer is positive and lead Vogel [296] to the following result: let $\mathcal{H}$ be a Hilbert space and let $\hat{H} = \sum_n E_n |\phi_n\rangle\langle\phi_n|$ be a Hamiltonian with pure point spectrum and several other properties (relevant for the exact result), including for instance the number of distinct eigenvalues of $\hat{H}$, the maximal degeneracy of eigenvalues of $\hat{H}$ and other properties concerning the gaps of $\hat{H}$ (see [296] for details). Further let $\hat{B}$ be a bounded operator on $\mathcal{H}$. It can be shown that most $\psi_0 \in \mathbb{S}(\mathcal{H})$ with respect to $\text{GAP}_{\hat{\rho}}$ are such that for most $t \geq 0$ (in the long run) and under further conditions not important here (see [296] for details)

$$\langle\psi_t|\hat{B}|\psi_t\rangle \approx M_{\hat{\rho}\hat{B}} \quad (10.35)$$

with the deterministic approximation

$$M_{\hat{\rho}\hat{B}} = \sum_n \langle\phi_n|\hat{\rho}|\phi_n\rangle \langle\phi_n|\hat{B}|\phi_n\rangle. \quad (10.36)$$

Notice that generalized normal typicality is obtained for $\hat{B} = \hat{P}_\nu$ and $\hat{\rho} = \hat{P}_{\nu'}/d_{\nu'}$.

We mention this here for several reasons: first, it fits in nicely to the discussion of GAP measures. Second it's another instance of typical behavior in the BQF and also supports the individualistic view. Third, it points at equivalence of ensembles. As discussed above equivalence of ensembles means more or less that it doesn't matter which ensemble one chooses. As the GAP measures are analogs of the Gibbs ensembles, the result just stated is another instance of this equivalence as generalized normal typicality (10.35) occurs for all the relevant ensembles (for more details see [278]).

11. Ensemble Justification

Following [136] and [175, Sec.7.1] we argue that ensembles are best understood in the context of typicality and not genuine probability (see also [9, 34, 121]). As a consequence thermal equilibrium does not rely on the knowledge of an observer, but is simply a fact appearing in nature.

This reasoning relies on canonical typicality, which informally means the following: most wave functions Ψ from the energy shell are such that

$$\mathrm{tr}^B |\Psi\rangle\langle\Psi| \approx \hat{\rho}_{\mathrm{can}}, \quad (11.1)$$

given that S and B are weakly coupled, while B is large enough. This follows from a law-of-large type number argument and legitimates the appearance of the canonical density matrix.

Our line of thought here goes like this: in Section 11.1 we explain ensemble typicality and in Section 11.2 we criticize views justifying ensembles relying on “subjective” interpretations of probability.

11.1. Ensemble Typicality

Ensemble typicality is a justification for the use of ensembles and is based on canonical typicality [133, 214] (see [219] for similar reasoning) and in particular [177, Sec.9]. We consider a system S and a heat bath B with corresponding Hilbert spaces $\mathcal{H}^S$ (with $\dim \mathcal{H}^S = d_S$) and $\mathcal{H}^B$ (with $\dim \mathcal{H}^B$) and let $\mathcal{H}_{\mathrm{mc}} \subset \mathcal{H}^S \otimes \mathcal{H}^B$ be the micro-canonical energy shell. Canonical typicality provides that most $\Psi \in \mathbb{S}(\mathcal{H}_{\mathrm{mc}})$ and $\hat{A} \in \mathcal{A}_{\mathrm{MITE}}$ (see Section 9.3), i.e., observables of the form $\hat{A} = \hat{A}^S \otimes \hat{I}^B$, are such that

$$\langle\Psi|\hat{A}|\Psi\rangle \approx \mathrm{tr}(\hat{\rho}_{\mathrm{mc}}\hat{A}) \quad (11.2)$$

for sufficiently large B . As a consequence a single pure state provides the same statistics as the micro-canonical density matrix $\hat{\rho}_{\mathrm{mc}}$. In our view that is a justification for $\hat{\rho}_{\mathrm{mc}}$ in a conceptually unproblematic manner. At the same time it’s also a justification for the other ensembles, since they can be derived from $\hat{\rho}_{\mathrm{mc}}$. We elaborate different aspects of this below and in Appendix 11.2.

Goldstein et al. [133] derived canonical typicality, based on thoughts by Schrödinger in 1952 [241]. Other approaches are due to Lloyd [184], Tasaki [269] and later Gemmer

and Mahler [108] and Popescu, Short and Winter [214]; a justification for the micro-canonical ensemble similar in spirit is [266].

While the canonical density matrix follows on average for $\Psi \sim u_{\mathbb{S}(\mathcal{H}_{\text{mc}})}$

$$\mathbb{E} \operatorname{tr}^B |\Psi\rangle\langle\Psi| = \operatorname{tr}^B \mathbb{E} |\Psi\rangle\langle\Psi| \quad (11.3)$$

$$= \operatorname{tr}^B \int_{\mathbb{S}(\mathcal{H}_{\text{mc}})} u(d\psi) |\psi\rangle\langle\psi| \quad (11.4)$$

$$= \operatorname{tr}^B \hat{\rho}_{\text{mc}} \approx \hat{\rho}_{\text{can}}, \quad (11.5)$$

where the last line follows from a standard textbook argument (see below), canonical typicality is stronger as $\operatorname{tr}^B \hat{\rho}_{\text{mc}}$ does not only appear on average, but it is shown that for sufficiently large B fluctuations around the average are negligible.

We now present the argument of Goldstein et al. [133], which builds on the law of large numbers. They argue that for most $\Psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ and B large enough,

$$\operatorname{tr}^B |\Psi\rangle\langle\Psi| \approx \hat{\rho}_{\text{can}}. \quad (11.6)$$

A key in their argument is that a uniformly distributed $\Psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ in high dimension can arise from a complex Gaussian vector in the following way: for $\Psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$ define

$$\Psi = \frac{\varphi}{\|\varphi\|} \quad (11.7)$$

with $\varphi \in \mathcal{H}_{\text{mc}}$ a complex Gaussian random vector with mean zero and covariance matrix $\mathbf{1}_{\text{mc}}$ (just the identity on $\mathcal{H}_{\text{mc}}$). Decomposing the vector φ in the eigenbasis of system and bath yields (same notation for eigenvectors as above (9.31) in Section 9.2) one gets

$$\varphi = \sum_i \sum_j c_{ij} |\phi_i^S\rangle |\phi_j^B\rangle, \quad (11.8)$$

where c_{ij} are complex Gaussian random variables. Further denote

$$\varphi = \sum_i |\phi_i^S\rangle |\varphi_i\rangle \quad (11.9)$$

with

$$|\varphi_i\rangle = \sum_{j \in I_i} c_{ij} |E_j^B\rangle. \quad (11.10)$$

Here I_i is the set of bath energy levels j , such that $E_j^B \in [E - E_i^S - \Delta E, E - E_i^S]$.

With this one computes the reduced density matrix

$$\hat{\rho}_{\Psi}^S = \text{tr}^B |\Psi\rangle\langle\Psi| = \frac{1}{\|\varphi\|^2} \text{tr}^B |\varphi\rangle\langle\varphi| \quad (11.11)$$

$$= \frac{1}{\|\varphi\|^2} \sum_{k,l} \langle\varphi_k|\varphi_l\rangle |\phi_k^S\rangle\langle\phi_l^S| \quad (11.12)$$

$$= \frac{1}{\|\varphi\|^2} \sum_i \|\varphi_i\|^2 |\phi_i^S\rangle\langle\phi_i^S|. \quad (11.13)$$

Using that $\|\varphi_i\|^2 = \sum_j |c_{ij}|^2$ and the fact that

$$\mathbb{E} \sum_j |c_{ij}|^2 = \dim(\mathcal{H}_i^B) \quad \text{and} \quad \|\varphi\|^2 = D \quad (11.14)$$

one finds with the law of large numbers that

$$\hat{\rho}_{\Psi}^S = \frac{1}{D} \sum_i \dim(\mathcal{H}_i^B) |\phi_i^S\rangle\langle\phi_i^S|. \quad (11.15)$$

Since $\dim(\mathcal{H}_i^B) \propto e^{-\beta E_i^S}$ it follows that $\hat{\rho}_{\Psi}^S$ is typically close to (9.31).

A more mathematically precise version of canonical typicality is the following [128, 284, 266]: let u_{mc} be the uniform distribution on $\mathbb{S}(\mathcal{H}_{\text{mc}})$. Then for arbitrary $\varepsilon > 0$,

$$u_{\text{mc}} \{ \Psi \in \mathbb{S}(\mathcal{H}_{\text{mc}}) : \|\text{tr}^B |\Psi\rangle\langle\Psi| - \text{tr}^B \hat{\rho}_{\text{mc}}\|_{\text{tr}} < \varepsilon \} \geq 1 - \frac{d_S^4}{\varepsilon^2 D}. \quad (11.16)$$

Hence if $d_S \ll \varepsilon^{1/2} D^{1/4}$, then for most $\Psi \in \mathbb{S}(\mathcal{H}_{\text{mc}})$, the reduced density matrix $\text{tr}^B |\Psi\rangle\langle\Psi|$ is close to $\text{tr}^B \hat{\rho}_{\text{mc}}$ (in the sense of the trace norm⁵³); for a proof see [284, 266].

Popescu, Short and Winter [214] consider the following setup. As usual let $\mathcal{H} = \mathcal{H}^S \otimes \mathcal{H}^B$. Now, different to the above derivation instead of $\mathcal{H}_{\text{mc}}$, they consider a global constraint on the total system, leading to the subspace $\mathcal{H}^R \subseteq \mathcal{H}$ with $\dim \mathcal{H}^R = d_R$. They assign to it a density matrix $\hat{\rho}^R = \hat{P}_R/d_R$ with projector $\hat{P}_R$ onto $\mathcal{H}^R$. Then for most $\Psi \in \mathbb{S}(\mathcal{H}^R)$

$$\text{tr}^B |\Psi\rangle\langle\Psi| \approx \text{tr}^B \hat{\rho}^R. \quad (11.17)$$

Their proof relies on Levy's lemma, for which different versions exist (for a more elaborate discussion see [279]). Here's a version that is enough for our purposes as it

⁵³For an operator $\hat{A}$ on $\mathcal{H}$ the trace norm is given by $\|\hat{A}\|_{\text{tr}} = \text{tr} \sqrt{\hat{A}^* \hat{A}}$.

illustrates another instance of a typicality statement.

Let $\mathcal{H}$ be a finite dimensional Hilbert space with dimension D . Let $f : \mathbb{S}(\mathcal{H}) \rightarrow \mathbb{R}$ be a Lipschitz continuous function with Lipschitz constant η and let $u_{\mathbb{S}(\mathcal{H})}$ be the uniform area measure on $\mathbb{S}(\mathcal{H})$. Then for $\varepsilon > 0$ the following holds

$$u_{\mathbb{S}(\mathcal{H})} \left\{ \psi \in \mathbb{S}(\mathcal{H}) : |f(\psi) - u(f)| > \varepsilon \right\} \leq 4 \exp \left(-\frac{2D\varepsilon^2}{9\pi^3\eta^2} \right), \quad (11.18)$$

where $u(f) = \int_{\mathbb{S}(\mathcal{H})} f(\psi) u(d\psi)$. Stated differently: most points on a high dimensional sphere are such that (Lipschitz) continuous functions are approximately constant. This is another property of spheres in high dimensions related to concentration of measure phenomena (see Section 3.1).

Canonical typicality holds for wave functions that are distributed uniformly on the energy shell. A natural question is whether that can be extended to other measures μ on the unit sphere, such that a similar statement can be made. It turns out that this is the case for GAP measures. One can show that for $\hat{\rho}$ on $\mathcal{H}$ with small eigenvalues, GAP $_{\hat{\rho}}$ -most $\psi \in \mathbb{S}(\mathcal{H}^S)$ are such that [278]

$$\hat{\rho}_{\psi}^S \approx \text{tr}^B \hat{\rho}. \quad (11.19)$$

More precisely, for any $\varepsilon > 0$:

$$\text{GAP}_{\hat{\rho}} \left\{ \psi \in \mathbb{S}(\mathcal{H}) : \|\hat{\rho}_{\psi}^S - \text{tr}^B \hat{\rho}\|_{\text{tr}} > \varepsilon \right\} \leq 6d_S^2 \exp \left(\frac{-C\varepsilon^2}{d_S^2 \|\hat{\rho}\|} \right) \quad (11.20)$$

where $C = 1/1152\pi^2$ and $\|\hat{\rho}\|$ the operator norm of $\hat{\rho}$. Let us mention that generalized canonical typicality is not “only” (as the proof is quite involved) a mathematical extension of canonical typicality. Levy’s lemma has to be adjusted in a non-trivial way to GAP measures [214]: let $\mathcal{H}$ be a separable Hilbert space, $f : \mathbb{S}(\mathcal{H}) \rightarrow \mathbb{R}$ with Lipschitz constant η , let $\hat{\rho}$ be a density matrix on $\mathcal{H}$. Then for $\varepsilon > 0$:

$$\text{GAP}_{\hat{\rho}} \left\{ \psi \in \mathbb{S}(\mathcal{H}) : |f(\psi) - \text{GAP}_{\hat{\rho}}(f)| > \varepsilon \right\} \leq 6 \exp \left(\frac{-C'\varepsilon^2}{\eta^2 \|\hat{\rho}\|} \right) \quad (11.21)$$

where $C' = 1/288\pi^2$. For other statements and proofs we refer to [278]. Here we focus especially on the conceptual consequences of “GAP canonical typicality”.

As the actual distribution of the wave function might not be uniform, the result shows that this is not needed (at least quite, it can also not be to non-uniform). This is interesting from two points of view: first, density matrices arise as statistical operators, as a consequence of being sampled according to some distribution μ . And second, the GAP measure serves as *typicality* measures. Here no sampling is needed

as the typical behavior refers to instances that happen in most cases. Further it turns out that the cutoff in the micro-canonical energy shell $[E - \Delta E, E]$ is not important. Any old ψ does the job (see [279] for more details).

It also sheds light on equivalence of ensembles, which says that it does not really matter which ensemble one uses.

This can be made precise; it follows from generalized canonical typicality for GAP measures. Suppose two systems S and B interact weakly and B is large enough. Then $\hat{\rho}_{\text{mc}}$ and $\hat{\rho}_{\text{can}}$ on $\mathcal{H} = \mathcal{H}^S \otimes \mathcal{H}^B$ both lead to $\hat{\rho}_{\text{can}}^S$ in $\mathcal{H}^S$ namely via

$$\text{tr}^B \hat{\rho}_{\text{mc}} \approx \hat{\rho}_{\text{can}}^S \approx \text{tr}^B \hat{\rho}_{\text{can}} \quad (11.22)$$

given suitable values of β in $\hat{\rho}_{\text{can}}$ and $\hat{\rho}_{\text{can}}^S$ for energy E of $\hat{\rho}_{\text{mc}}$. That means that by generalized canonical typicality (11.20) one can compute either $\text{GAP}_{\hat{\rho}_{\text{mc}}} = u_{\text{mc}}$ or $\text{GAP}_{\hat{\rho}_{\text{can}}}$ and get for both that most ψ are such that $\hat{\rho}_{\psi}^S$ is approximately constant or roughly canonical.

Further interesting statements about the time evolution can be made. These are connected to dynamical typicality. Briefly put this means that for typical wave functions the time evolution has the same look. More precisely for $\text{GAP}_{\hat{\rho}}$ -most ψ and most $t \in [0, T]$

$$\hat{\rho}_{\psi_t}^S \approx \text{tr}^B \hat{\rho}_t \quad (11.23)$$

with $\hat{\rho}_t = \exp(-i\hat{H}t)\hat{\rho}_0 \exp(i\hat{H}t)$. To mention here is that a general density matrix evolves in time, while the micro-canonical density matrix (and under certain conditions usually satisfied also the other standard TD ensembles) is invariant under time evolution. The uniform distribution is invariant under time evolution, but $\text{GAP}_{\hat{\rho}_0}$ is not. For $\psi_0 \sim \text{GAP}_{\hat{\rho}_0}$ and for every $\varepsilon, T > 0$ with $\|\hat{\rho}\| < 1/4$:

$$\text{GAP}_{\hat{\rho}} \left\{ \psi \in \mathbb{S}(\mathcal{H}) : \frac{1}{T} \int_0^T \|\hat{\rho}_{\psi_t}^S - \text{tr}^B \hat{\rho}_t\|_{\text{tr}} dt > \varepsilon \right\} \leq \frac{28d_S^3 \text{tr} \hat{\rho}^2}{\varepsilon}. \quad (11.24)$$

11.2. Probabilities and Ensembles

There are other ways of deriving ensembles in equilibrium statistical mechanics⁵⁴. As stated in the beginning of this thesis these justifications are misguided and already begin with asking the wrong question, namely

What is the probability distribution on the set of micro states in thermal equilibrium?

⁵⁴We can not discuss all of them in detail. Here we focus on two approaches, that are in opposition to our typicality view. In particular these views do not allow making objective statements about thermal properties of systems. The typicality account however does that.

When asking for a probability distribution one has already taken the wrong turn⁵⁵. The meaning of probabilities used to derive the ensembles are “objective”, in the sense of frequencies, or “subjective”, in the sense of ignorance (or degrees of belief) (see, e.g., [9, Sec. 8.1] or [34, Ch. 2]). However, we saw in the previous sections that ensembles are best understood in terms of typicality. Still “a skeptical mind”[34, p.171] could ask:

“What is so special about those distributions that being typical with respect to them has an explanatory value or counts as a justification for the equilibrium statistical formalism?”[34, p.171]

Well, from the perspective of typicality there is nothing left to explain. Once a phenomenon has turned out to be typical that’s it⁵⁶.

As the standard thermodynamic ensembles, such as the canonical or grand-canonical ensemble are derived from the micro-canonical ensemble, we will only discuss justifications of the micro-canonical ensemble. There are two prominent views to derive ensembles: the **principle of equal a priori probabilities (PEP)** and the **maximum entropy principle (MEP)**. Both approaches share a common “justification”⁵⁷, which relies on the empirical success of the theory. We will not discuss this any further as its a valid, but certainly not satisfactory justification (see [34, 151] for a detailed discussion). It is similar to asking why a car drives by showing that it does. Another point mentioned often in the literature (see, e.g., [34, 212]) is stationarity. It follows from the von Neumann equation that $\hat{\rho}$ has to commute with $\hat{H}$ and thus $\hat{\rho}$ is a roughly said a function of energy (think of $\hat{\rho} \propto \exp(-\beta\hat{H})$). Let us just mention that there is another proposal by Oliver Penrose [211, 212] that does not rely on the PEP and MEP (also critisizing these views). Ensemblism should be regarded as a practical tool and not be considered fundamental.

Principle of Equal a Priori Probability

Here’s a guiding (or fundamental) principle stated in common textbooks (see, e.g. [146, 243, 157, 280, 39, 247]) on statistical physics in order to justify the micro-canonical ensemble, first stated by Tolman [281, §23]⁵⁸:

Principle of Equal a Priori Probability (PEP): For a closed system in thermal equilibrium with certain macroscopic constraints, each micro state is equally probable compatible with those constraints.

⁵⁵This might be to exageratting. What we mean is this: the question is ultimately related to the meaning of probability as the derivation of ensembles is.

⁵⁶So the skeptical mind should go back to Section 3.1.

⁵⁷Albeit being principles, they do not rely on any further assumptions, they just make it work.

⁵⁸Historically a similar thought goes back to Boltzmann maybe more related to the ergodic hypothesis [181, p.92]

Given the constraint that the energy of the system lies in the interval $[E - \Delta E, E]$ the PEP leads to the micro-canonical density matrix

$$\hat{\rho}_{\text{mc}} = \frac{\hat{P}_{\text{mc}}}{D}, \quad (11.25)$$

where $\hat{P}_{\text{mc}}$ is the projector onto $\mathcal{H}_{\text{mc}}$, the spectral subspace of $\hat{H}$ spanned by eigenvectors with eigenvalues in $[E - \Delta E, E]$.

The PEP has its roots in the “indifference principle” of Keynes [160, Ch.4], which is an extension of Bernoulli’s “principle of insufficient reason” [19] (see, e.g., [244, 211, 212, 10, 8]). If there is no reason to treat any of the possible states differently, then all have the same probability (think of a dice).

We find the PEP not satisfactory. We think it’s not a rational guess that is decisive, but the fact that thermal equilibrium is typical. Why should thermal equilibrium depend on a rational guess? What determines a rational guess? Why can the principle of indifference applied here after all?

The PEP can be extended to the maximum entropy principle to which we come next. This makes heavy use of the knowledge of an observer, which can also be (but must not be; for a frequentist understanding of the PEP see [281, Ch.24] and [212]) seen in the PEP. Here’s, for instance Jancel:

“In order to conclude the determination of this representative ensemble, we must define a probability density for it: thus, an essentially statistical hypothesis must be made concerning the *a priori* probabilities appropriate to the various states of the system compatible with our knowledge.”[151, P.10]

or Balian

“[...] if we do not know anything about a system it is natural to represent it by the statistical ensemble which is *completely disordered*, where the probabilities of the $W[D, C.I.]$ possible micro-states are equal.[11, p.142]”.

Again, thermal equilibrium does not depend on our knowledge. If we, as Balian says, know nothing, then we do know nothing, but still thermal equilibrium is there and our knowledge has nothing to do with that.

Maximum Entropy Principle

Another justification of ensembles is the maximum entropy principle (see, e.g., [163, 189, 112, 173]), which dates back to Gibbs [115] (see also Tolman [281, §29]) and has been prominently developed by Jaynes [153, 152] on the basis of works of Shannon [248]. It can be regarded as an extension of the principle of indifference and interprets the von Neumann or the Gibbs entropy as “uncertainty” or “missing information”. In thermal equilibrium this uncertainty should be maximal given all the relevant information one has about a system. More precisely [11, Sec. 4.1.3]

Maximum entropy principle (MEP): Among those density matrices $\hat{\rho}$ on $\mathcal{H}$ compatible with the available data we must represent the system by that macro state which has maximal statistical entropy $S(\hat{\rho})$.

The MEP is a general answer to the “wrong” question in the beginning of this chapter. It yields one principle, is simple, elegant and captures a lot of cases (see, e.g., [34, Ch. 7] and [212, p.1943]). Let us state the procedure stemming from the MEP. We follow [11] and focus on the quantum case. Let $\hat{\rho}$ be a density matrix on a Hilbert space $\mathcal{H}$ with dimension $\dim \mathcal{H} = D$. The statistical entropy is just the von Neumann entropy

$$S_{\text{vN}}(\hat{\rho}) = -k_B \text{tr} \hat{\rho} \log \hat{\rho}. \quad (11.26)$$

Further let $\hat{M}_1, \dots, \hat{M}_K$ be a collection of self-adjoint operators on $\mathcal{H}$. Among the “available data” are the expectation values M_i

$$\text{tr}(\hat{\rho} \hat{M}_i) = M_i \quad \forall i \in [K], \quad (11.27)$$

$$\text{tr}(\hat{\rho}) = 1. \quad (11.28)$$

Using the Lagrange multiplier method the maximum of (11.26) under the constraints (11.27) is given by the equilibrium density matrix

$$\hat{\rho}_{\text{eq}} = \frac{1}{Z} \exp \left(\sum_{i=1}^K \lambda_i \hat{M}_i \right). \quad (11.29)$$

Here $\lambda_1, \dots, \lambda_K$ are Lagrange multipliers, while Z is a normalization constant. It can be shown that (11.29) is indeed a minimizer for (11.26) [11, Sec. 4.2.2]; note that we have discussed this above in the setting of the generalized Gibbs ensembles. Let us remark here that the results we obtained in 11.2 justify these ensembles via typicality reasoning. The MEP however can not do this. We will now say why.

We think the MEP is unsatisfactory for several reasons (for further critique see, e.g., [40, 174, 126, 121]). These rely mostly on the use of “information”, “data” or knowledge in the MEP (as mentioned at several instances in this thesis) and the choice of entropy, which is the Gibbs (or Shannon) entropy and its misinterpretation with thermodynamic entropy.

The most important one is that thermal equilibrium has nothing to do with the ignorance or the knowledge of an observer about a system. If one is appealing to the notion of an observer, the consequence is that in the absence of an observer could not be applied for realistic cases. Does the cup of coffee in the office next to an observer thermalize or not? Does it get cold in winter time if I’m unsure whether I left the window in my appartement open or not? That is the significance of the MEP for physics is not clear at all. The MEP relies on understanding statistical physics as a

kind of statistical interference and not a description of reality [212, p.1943]. Here's Jaynes himself:

“[It] is not a physical theory, but a form of statistical inference [...] instead of seeking the unattainable [it] asks a more modest question: ‘Given the partial information that we do in fact have, what are the best predictions we can make of observable phenomena?’”[154, p.416]

If it's not a physical theory, but aims at making the correct predictions about a physical system, what should it then be? We believe that the modesty of Jaynes is not honest. One can argue what the essence of thermal equilibrium is and one should have the guts to do that. Then one can be modest about the fact that there is regularity and beauty in nature that can be captured by humans still being independent of them.

With respect to subsystems we have argued in Appendix 11.2 and also above in Section 11.1 that there is nothing subjective about $\text{tr}^B |\Psi\rangle\langle\Psi|$. Once it has been coined typical there is nothing left to explain. And ensemble typicality shows exactly that. We have seen that ensembles simply occur in nature.

And further why is no other data relevant? (see [212, p.1943]) A possible conclusion is that one can find with the MEP what one already knows, but with reliance on knowledge or subjectivity. Further we do not see average, but the typical behavior of a system. That is what happens in most instances [34, Sec. 7.8].

Another reason to say that thermal equilibrium has nothing to do with the MEP is this. Can different observers have different informations? In this case would it be possible to draw the same conclusions? [136, p.14] Further suppose that one is considering an irrational observer, who is not capable of collecting the information needed or simply does not care. Would you rely on such a person, telling you that he found out that this cup of coffee is drinkable? Further: what defines a rational observer? All these questions show that there is a lot of doubt to think that an observer plays any role for the thermal equilibrium properties of a system.

Further it is mentioned by Penrose that the statistical inference approach leads to paradoxical results (see [212, p.1943] and the cited references therein). That is in general it's not easy to see which subjective probability one should assign to an event given certain data (not those in the MEP, which are constructed by design to yield the thermodynamic outcomes) [34, Sec.2.2.4]; let us just mention that such an example is given by Bertrand's paradox (see [34, Sec.2.2.5]).

There is another common objection to the MEP pinned down to the phrase: “ex nihilo nihil”. It means that it is not possible to anything out of the knowledge of our ignorance [56]. Or stated differently: “Unperformed experiments have no results” (see [213]). In principle the MEP reproduces what one already knows. That has to do

with the question asked at the beginning of this chapter. It is phrased in such a way that the MEP is the fitting answer to it. But it turns out that this lacks a wrong understanding about the status of probability for thermodynamic ensembles.

Another common argument against the MEP is that standard thermodynamic results depend on the choice of variables, which hints at a similar point just made, namely that with the MEP one just wants to show what one already knows (see [56] for this argument).

The MEP makes use of data or knowledge or information. But as pointed out by Bricmont [34, Sec.7.8] “information [...] is always information about something different from itself”. There is a way to quantify information, but say the same chunk of information can be very differently for our everyday life. But science should not be about information. And similar as the ensemblistic view one can consider information theoretical approaches in science as a tool, but these are not the end of the story.

Here’s another thought related to our actions. Mostly we are not in laboratory situations where it seems that the MEP fits best (so the MEP might be itself an idealization of a situation that never really occurs). Usually we find thermal behavior in our everyday life and commonly we do not use the MEP to be certain whether a cup of coffee has cooled down such that we can drink it without harming ourselves. The point we want to make is that there are facts in nature happening that don’t depend on the knowledge we have or that we don’t have. And these can have severe consequences for our actions and even for our lives. Gas spreads out in a room and that does not depend on what we know or don’t know.

So why are people appealing to subjective entropy at all? The justification for its use as a principle is also by its empirical success [11, p.145] and as mentioned above it captures a lot of cases and its simple and elegant. Further, since probability distributions are commonly used in classical mechanics, one can extend the notion to quantum mechanics and express the system’s state by a density matrix. This stems from a wrong conclusion drawn from the insight that a many particle system has to be considered from a probabilistic point of view. For the ensemblist this means that probability is meant as subjective probability, that is the lack of knowledge ones has about a system. Another possibility to consider a subjective point of view is due to the standard formulation of quantum mechanics, where the role of the observer is key in the collapse postulate. The entropy considered in the MEP is thought of as a measure quantifying this lack of knowledge. It has its roots in Shannon entropy [152]. This analogy is however misleading as Shannon was concerned with the transmission of data and not with thermodynamic entropy [136]. A last reason to stick with the MEP is that objective entropy “either does not work or is ugly”[136, p.16].

The upshot is that ensemble typicality is stronger than the MEP and that the

“study of subjective entropy is a subfield of psychology, not of physics. It is all

about beliefs. Some ensemblists may be inclined to say that the explanation of heat flow is that it occurs the same way as *if* an observer observed it. But the fact remains that observers actually have nothing to do with it.”[p.14][136]

Remark 11.2.1. We have seen that ensembles can be understood in terms of typicality. Still the most prominent justification of the ensembles is based on the MEP. This relies heavily on subjective notions such as knowledge or data or information. While the roots of ensemblism go back all the way to Maxwell [181] they are usually related to Gibbs [115]. Certainly both Maxwell and Gibbs did not consider themselves ensemblists or relied on subjective elements being relevant to physics. Thus it would of interest to dig deeper and try to find out where and why subjectivity entered physics? There are some starting points one can consider, for instance the paper by the Paul and Tatjana Ehrenfest [87] from 1912 or the paper by Leó Szilárd on Maxwell’s demon [267] from 1929. It is also apparent that the developement of OQM which relies so much on an observer and thus on subjectivity might have had an influence on the considerations of Szilárd or the advocates of ensemble theory discussed above. Further it would be of interest to see how social dynamics have influenced physics, for instance during the Weimar republic in the 1920s [14, 71] and also subjective elements in statistical physics in the postmodern area [32]. $\diamond$

Ensemble typicality makes a case why systems are in thermal equilibrium in an objective manner and that is because its typical and that is all there is.

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Appendix

Submitted Manuscripts

Grand-Canonical Typicality

Grand-Canonical Typicality

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Abstract

We study how the grand-canonical density matrix arises in macroscopic quantum systems. “Canonical typicality” is the known statement that for a typical wave function Ψ from a micro-canonical energy shell of a quantum system S weakly coupled to a large but finite quantum system B , the reduced density matrix $\hat{\rho}_{\Psi}^S = \text{tr}^B |\Psi\rangle\langle\Psi|$ is approximately equal to the canonical density matrix $\hat{\rho}_{\text{can}}^S = Z_{\text{can}}^{-1} \exp(-\beta \hat{H}^S)$. Here, we discuss the analogous statement and related questions for the *grand-canonical* density matrix $\hat{\rho}_{\text{gc}}^S = Z_{\text{gc}}^{-1} \exp(-\beta(\hat{H}^S - \mu_1 \hat{N}_1^S - \dots - \mu_r \hat{N}_r^S))$ with $\hat{N}_i^S$ the number operator for molecules of type i in the system S . This includes (i) the case of chemical reactions and (ii) that of systems S defined by a spatial region which particles may enter or leave. It includes the statements (a) that the density matrix of the appropriate (generalized micro-canonical) Hilbert subspace $\mathcal{H}_{\text{gmc}} \subset \mathcal{H}^S \otimes \mathcal{H}^B$ (defined by a micro-canonical interval of total energy and suitable particle number sectors), after tracing out B , yields $\hat{\rho}_{\text{gc}}^S$; (b) that typical Ψ from $\mathcal{H}_{\text{gmc}}$ have reduced density matrix $\hat{\rho}_{\Psi}^S$ close to $\hat{\rho}_{\text{gc}}^S$; and (c) that the conditional wave function ψ^S of S has probability distribution $\text{GAP}_{\hat{\rho}_{\text{gc}}^S}$ if a typical orthonormal basis of $\mathcal{H}_B$ is used. That is, we discuss the foundation and justification of both the density matrix and the distribution of the wave function in the grand-canonical case. We also extend these considerations to the so-called generalized Gibbs ensembles, which apply to systems for which some macroscopic observables are conserved.

Key words: thermal density matrix; chemical equilibrium; chemical potential μ ; generalized Gibbs ensemble; GAP measure; conditional wave function.

1 Introduction

We are concerned with quantum analogs of the micro-canonical, the canonical, and the grand-canonical ensemble introduced by Gibbs [10] to classical statistical mechanics. While the micro-canonical and the canonical ones have been discussed extensively in

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the literature, we cover here the foundations of the grand-canonical one (as well as the generalized Gibbs ensemble of (7) below). Each of the three ensembles has two kinds of analogs in quantum theory: a density matrix and a probability distribution of wave functions (i.e., over the unit sphere in Hilbert space). The density matrices are well known:

$$\hat{\rho}_{\text{mc}} = Z_{\text{mc}}^{-1} \mathbb{1}_{[E-\Delta E, E]}(\hat{H}) \quad (1a)$$

$$\hat{\rho}_{\text{can}} = Z_{\text{can}}^{-1} \exp(-\beta \hat{H}) \quad (1b)$$

$$\hat{\rho}_{\text{gc}} = Z_{\text{gc}}^{-1} \exp\left(-\beta(\hat{H} - \mu_1 \hat{N}_1 - \dots - \mu_r \hat{N}_r)\right) \quad (1c)$$

are the micro-canonical, canonical, and grand-canonical density matrices of a quantum system with Hamiltonian $\hat{H}$ and, in the last case, particle number operator $\hat{N}_i$ for particle type $i = 1, \dots, r$; Z is always the normalizing constant, β the inverse temperature, μ_i the parameter called the chemical potential, and $\mathbb{1}_{[E-\Delta E, E]}(\hat{H})$ is the projection to the energy shell or micro-canonical subspace $\mathcal{H}_{[E-\Delta E, E]} \subset \mathcal{H}$ (i.e., the spectral subspace of $\hat{H}$ for this interval, or the span of all eigenvectors with eigenvalue in this interval) in the Hilbert space $\mathcal{H}$. It is assumed in (1c) that

$$\left[\hat{H}, \sum_i \mu_i \hat{N}_i\right] = 0, \quad (2)$$

or else $\hat{\rho}_{\text{gc}}$ would not be invariant under the unitary time evolution $\exp(-i\hat{H}t/\hbar)$ and thus not represent thermal equilibrium (a stationary state).

The relevant distribution of the wave function in the unit sphere

$$\mathbb{S}(\mathcal{H}) = \{\psi \in \mathcal{H} : \|\psi\| = 1\} \quad (3)$$

of $\mathcal{H}$ is [58, 19]

$$\mathbb{P}_{\text{mc}}(d\psi) = u_{\mathbb{S}(\mathcal{H}_{[E-\Delta E, E]})}(d\psi) \quad (4a)$$

$$\mathbb{P}_{\text{can}}(d\psi) = \text{GAP}_{\hat{\rho}_{\text{can}}}(d\psi) \quad (4b)$$

in the micro-canonical and canonical case, where $u_{\mathbb{S}}$ means the normalized uniform distribution over the sphere $\mathbb{S}$ (i.e., the surface area measure such that $u_{\mathbb{S}}(\mathbb{S}) = 1$) and $\text{GAP}_{\hat{\rho}}$ the GAP measure [25, 19, 17, 50, 31, 56, 32, 33] with density matrix $\hat{\rho}$ (i.e., the most spread-out measure with density matrix $\hat{\rho}$, see Section 7.1 for the definition). Among other things, we determine $\mathbb{P}_{\text{gc}}$ in this paper (see Statements 3 and 4b in Section 3).

The justification of the canonical and grand-canonical density matrices and distributions of wave functions has to do with weakly coupling the quantum system, let us call it S , to another quantum system B that is much bigger than S (but finite) and serves as a bath (reservoir). There is then a precise sense in which a particular probability distribution on $\mathbb{S}(\mathcal{H}^S)$ (where we write the system as an upper index) is “the correct” distribution: this sense is that it agrees with the typical distribution of the *conditional wave function* [27, 5, 8, 19, 50], a concept first introduced in Bohmian mechanics [27, 5] but applicable in any version of quantum mechanics; see Section 3 for the definition

and discussion. Put briefly, the conditional wave function of a system S entangled with another system B is defined using an orthonormal basis $b = \{|b_1\rangle, |b_2\rangle, \dots\}$ of $\mathcal{H}^B$ and represents the random wave function that one would obtain for S if one carried out on B an ideal quantum measurement corresponding to b .

There are two well-known ways of justifying $\hat{\rho}_{\text{can}}$: either as the partial trace over B of the micro-canonical density matrix of $S \cup B$, or as the partial trace over B of $|\Psi\rangle\langle\Psi|$, where the wave function Ψ of $S \cup B$ is a typical unit vector in the micro-canonical subspace of $\mathcal{H}^S \otimes \mathcal{H}^B$ (a consideration known as *canonical typicality* [9, 36, 18]). Since the former density matrix is the average of the latter, the latter argument is the stronger one: it asserts that for *most* Ψ , S will appear to have density matrix $\hat{\rho}_{\text{can}}$, whereas the former argument yields $\hat{\rho}_{\text{can}}$ for S only *on average*. These two ways arise as well in the grand-canonical case. For some of our statements, known results intended for $\hat{\rho}_{\text{can}}$ (such as [36, 17]) can as well be applied to $\hat{\rho}_{\text{gc}}$; other statements require new considerations.

In particular, our considerations are in line with the “individualist” attitude [13, 20] that a closed system $S \cup B$ in a pure state Ψ can display thermodynamic behavior; this attitude has been widely applied in recent years, in particular in connection with the eigenstate thermalization hypothesis (ETH) (e.g., [46, 30, 15, 12, 34]).

A standard way of arriving at either $\hat{\rho}_{\text{can}}$ or $\hat{\rho}_{\text{gc}}$ is to maximize the von Neumann entropy

$$S_{\text{vN}} = -k_{\text{B}} \text{tr}(\hat{\rho} \log \hat{\rho}) \quad (5)$$

(with Boltzmann’s constant k_{B}) under the constraint that the expected energy is fixed, $\text{tr}(\hat{\rho} \hat{H}) = E$ (as well as, in the grand-canonical case, the expected particle numbers, $\text{tr}(\hat{\rho} \hat{N}_i) = n_i$). While this reasoning may suggest that $\hat{\rho}_{\text{can}}$ ($\hat{\rho}_{\text{gc}}$) represents the knowledge of an observer who knows not more about the state than E (and n_i) (e.g., [24, 60], [1, Chap. 4], [2, Chap. 7]) the reasoning outlined above in terms of $S \cup B$ provides more [36]: a physical reason why the actual, physical state (of S) is given (approximately) by $\hat{\rho}_{\text{can}}$ (or $\hat{\rho}_{\text{gc}}$); see Section 4.1 for further discussion.

Also concerning the use of the micro-canonical distribution $u_{\text{mc}} = u_{\mathbb{S}(\mathcal{H}_{\text{mc}})}$ or density matrix $\hat{\rho}_{\text{mc}}$, there are different attitudes (e.g., [2, Sec. 6.8]) in the literature: Sometimes its use is regarded as a “principle of equal a priori probabilities” (e.g., [51, 23, 35]) saying that unless we have further knowledge about Ψ than that it lies in $\mathcal{H}_{\text{mc}}$, it is a rational guess to assign each point on $\mathbb{S}(\mathcal{H}_{\text{mc}})$ equal (subjective) probability. Our attitude is different: Since it is the nature of thermal equilibrium to behave like most Ψ , we find the thermal equilibrium behavior by studying the behavior of most Ψ , where “most” refers to u_{mc} (or, when appropriate, u_{gmc} over $\mathbb{S}(\mathcal{H}_{\text{gmc}})$ as in (8)).

Another aspect in the discussion of the grand-canonical ensemble arises from the fact that, already classically, there are two distinct situations in which it arises: (i) for chemical reactions such as



(“chemical equilibrium”), and (ii) when particles can enter and leave a system (defined by a region in space, “spatial equilibrium”). Many textbooks (e.g., [51, 28, 58, 44]) focus on spatial equilibrium when discussing the grand-canonical ensemble and omit

proper reasoning for chemical equilibrium, or focus on thermodynamic potentials when discussing chemical reactions and omit proper justification from the physical laws. Here, we provide this connection also for chemical equilibrium; we suggest that the latter is best understood by considering conserved macroscopic observables (such as $\hat{N}_A - \hat{N}_B$ and $\hat{N}_C + \hat{N}_A$ for the chemical reaction mentioned above) and the more abstract perspective of the so-called “generalized Gibbs ensemble” [1, (4.6)], [40, 3, 55, 34]

$$\hat{\rho}_{\text{gG}} = Z_{\text{gG}}^{-1} \exp \left(\sum_{k=1}^K \lambda_k \hat{Q}_k \right), \quad (7)$$

which we also discuss as it plays, in fact, a key role. It represents the thermal equilibrium ensemble for which $\hat{Q}_1, \dots, \hat{Q}_K$ (and only those) are conserved macroscopic observables,¹ assuming they commute with each other. (One of them usually is the Hamiltonian $\hat{H}$. Previous considerations in this direction can be found in [28, Sec. I.4].) Note that, as a consequence, there is a K -parameter family of thermal equilibrium states with parameters $\lambda_1, \dots, \lambda_K$ (which includes the canonical case with $K = 1$, $\hat{Q}_1 = \hat{H}$, and $\lambda_1 = -\beta$). The *generalized micro-canonical* subspace $\mathcal{H}_{\text{gmc}}$ for this situation is the one where the eigenvalues of each $\hat{Q}_k$ are restricted to an interval $[Q_k - \Delta Q_k, Q_k]$ that is short on the macroscopic scale but still has a high-dimensional spectral subspace $\mathbb{1}_{[Q_k - \Delta Q_k, Q_k]}(\hat{Q}_k) \mathcal{H}$,

$$\mathcal{H}_{\text{gmc}} := \text{span} \left\{ \phi \in \mathcal{H} : \forall k : \hat{Q}_k \phi = q_k \phi, q_k \in [Q_k - \Delta Q_k, Q_k] \right\} \quad (8a)$$

$$= \prod_{k=1}^K \mathbb{1}_{[Q_k - \Delta Q_k, Q_k]}(\hat{Q}_k) \mathcal{H}. \quad (8b)$$

We write

$$\hat{\rho}_{\text{gmc}} = \frac{\hat{P}_{\text{gmc}}}{\text{tr } \hat{P}_{\text{gmc}}} \quad (9)$$

for the normalized projection to $\mathcal{H}_{\text{gmc}}$. The key fact can now be formulated as follows:

General Gibbs Principle. *Suppose the self-adjoint operators $\hat{Q}_1, \dots, \hat{Q}_K$ commute with each other, and $\dim \mathcal{H}_{\text{gmc}}$ is large. Then, in relevant senses of equivalence of ensembles, $\hat{\rho}_{\text{gmc}}$ is equivalent to $\hat{\rho}_{\text{gG}}$ with λ_k chosen so that*

$$\text{tr}(\hat{\rho}_{\text{gG}} \hat{Q}_k) = Q_k. \quad (10)$$

(For $K = 1$ and $\hat{Q}_1 = \hat{H}$, we have that $\hat{\rho}_{\text{gc}} = \hat{\rho}_{\text{can}}$ and $\hat{\rho}_{\text{gmc}} = \hat{\rho}_{\text{mc}}$, and the general Gibbs principle asserts that the canonical density matrix is equivalent to the micro-canonical one, provided we define β through the relation $\text{tr}(\hat{H} e^{-\beta \hat{H}}) / \text{tr}(e^{-\beta \hat{H}}) = E$ with given energy E .)

¹The expression “macroscopic observable” is often intended to include the assumption that the eigenvalues of $\hat{Q}_k$ are separated by the resolution of macroscopic measurements; this is not intended here.

One relevant sense of equivalence is that, as conjectured by [3], they yield the same Born distribution for practically all observables $\hat{A}$ except very specially chosen functions of the $\hat{Q}_k$. We elucidate in Section 4.2 why this is plausible.

We focus on another sense: We say that for a composite system $S \cup B$, two density matrices $\hat{\rho}_1$ and $\hat{\rho}_2$ are *S-equivalent* if and only if

$$\mathrm{tr}^B \hat{\rho}_1 \approx \mathrm{tr}^B \hat{\rho}_2, \quad (11)$$

where tr^B means the partial trace over $\mathcal{H}^B$ and $\approx$ (for the sake of definiteness) closeness in the trace norm (but other senses of closeness could be considered as well). We define further that we call $\hat{\rho}_1$ and $\hat{\rho}_2$ *locally equivalent* if and only if for every sufficiently small spatial region S' , they are S' -equivalent. We conjecture that except for very special choices of $\hat{Q}_k$,

$$\hat{\rho}_{\mathrm{gG}} \text{ is locally equivalent to } \hat{\rho}_{\mathrm{gmc}}. \quad (12)$$

We can give here a derivation in the case in which each of the $\hat{Q}_k$ is (approximately) *extensive*, that is, in which, for any spatial region S and its complement $\bar{S}$,

$$\hat{Q}_k \approx \hat{Q}_k^S \otimes \hat{I}^{\bar{S}} + \hat{I}^S \otimes \hat{Q}_k^{\bar{S}}. \quad (13)$$

This is the first of our claims, see Statement 1a in Section 3. It includes the grand-canonical density matrix $\hat{\rho}_{\mathrm{gc}}$ as a special case (also for chemical equilibrium, see Section 2, but also for spatial equilibrium, where the conserved observables are simply $\hat{Q}_k = \hat{N}_k$).

We also discuss the *approach* (time evolution) toward the grand-canonical and the generalized Gibbs ensemble, both concerning the reduced density matrix and the distribution of the conditional wave function; we show that this approach occurs for every initial wave function if the Hamiltonian $\hat{H}$ satisfies the appropriate version of the eigenstate thermalization hypothesis (ETH), see Eq.s (65a) and (65b). For the reduced density matrix, we also prove a mathematical theorem (Proposition 2 in Section 8) that somewhat generalizes the existing results in this direction [47, 48, 39, 14, 34] (which were intended for the canonical density matrix). Concerning the approach to thermal equilibrium of the conditional wave function, no results have been in the literature before for either the canonical or the grand-canonical case.

A few words about the methods we employ: In some cases, the relevant “grand-canonical statements” can simply be obtained from known theorems that were intended for $\hat{\rho}_{\mathrm{can}}$ but apply to any high-dimensional subspace $\mathcal{H}_R \subset \mathcal{H}^S \otimes \mathcal{H}^B$, taken to be the micro-canonical subspace $\mathcal{H}_{\mathrm{mc}}$ defined by an energy interval for canonical typicality and taken here to be the generalized micro-canonical subspace $\mathcal{H}_{\mathrm{gmc}}$ defined by an energy interval *and* suitable intervals for the conserved observables $\hat{Q}_k$. Finally in other cases, some considerations specific to the grand-canonical case are required. Our derivations make particular use of theorems of Popescu et al. [36] and Goldstein et al. [17].

The remainder of this paper is organized as follows. In Section 2, we elucidate the framework that will also cover chemical reactions. In Section 3, we collect the main statements that we derive in this paper. In Section 4, we compare ours to other derivations. In Sections 5–8, we justify and discuss these statements.

2 Use of $\hat{\rho}_{\text{gc}}$: Chemical Reactions

While our statements in Section 3 also apply to spatial equilibrium, their full meaning unfolds itself in the case of chemical equilibrium. Since the latter is not commonly discussed in the way we treat it here, we first set the stage in this section by describing our perspective on the use of $\hat{\rho}_{\text{gc}}$ for chemical reactions. Specifically, we explain how the general Gibbs principle formulated around (10) can be applied here, yields $\hat{\rho}_{\text{gc}}$, and allows us to determine the chemical equilibrium. On that basis, we can then formulate our statements in Section 3.

Consider a macroscopic quantum system containing r different chemical substances $A_1, \dots, A_r$, and let n_i with $i = 1, \dots, r$ stand for the number of molecules of substance A_i . As a general version of (6), suppose there are $L \in \mathbb{N}$ possible chemical reactions, given by

$$\nu_{\ell 1} A_1 + \dots + \nu_{\ell r} A_r \rightleftharpoons \tilde{\nu}_{\ell 1} A_1 + \dots + \tilde{\nu}_{\ell r} A_r + \delta E_\ell \quad (14)$$

with $\ell = 1, \dots, L$, $\nu_{\ell i}, \tilde{\nu}_{\ell i} \in \{0, 1, 2, \dots\}$ the number of molecules A_i involved, and δE_ℓ the amount of energy (positive, negative, or possibly zero) released (or, if negative, consumed) in this reaction. Suppose initially the system contains n_{0i} molecules A_i for each $i = 1, \dots, r$ and has energy in the micro-canonical interval $[E - \Delta E, E]$. The questions arise:

$$\text{What are the numbers } n_{\text{eq},i} \text{ of } A_i \text{ in chemical equilibrium?} \quad (15)$$

And

$$\text{How can grand-canonical density matrices be used for calculating them?} \quad (16)$$

We answer both in this section. Our reasoning applies not only to chemical reactions but also to ionization and to elementary particle reactions.

The appropriate Hilbert space is

$$\mathcal{H} = \mathcal{F}_1 \otimes \dots \otimes \mathcal{F}_r \quad (17)$$

with

$$\mathcal{F}_i = \bigoplus_{n_i=0}^{\infty} \mathcal{F}_i^{(n_i)} \quad (18)$$

the Fock space of the molecules of type i and $\mathcal{F}_i^{(n_i)}$ the sector with n_i molecules; it is a fermionic (bosonic) Fock space whenever the number of fermions in the molecule is odd (even), which occurs for an electrically neutral molecule (i.e., one whose number of electrons equals the number of protons) whenever the number of neutrons per molecule is odd (even). (Note that the 1-particle Hilbert space $\mathcal{H}_i$ from which $\mathcal{F}_i$ arises may also involve internal degrees of freedom.)

Remark 1. There may be a (somewhat arbitrary) choice of the theoretical physicist involved in defining which states exactly count (say, in the example of (6)) as states of molecule C as opposed to states of a molecule A and a molecule B [29, Sec. 3]. We assume in the following that such a choice has been made. In the case of ionization (say,

$A = \text{proton}$, $B = \text{electron}$, $C = \text{hydrogen atom}$), a natural choice [11] would be to count the bound states (from the discrete spectrum of the relative Hamiltonian) as atoms C and the scattering states (from the continuous spectrum of the relative Hamiltonian) as $A + B$. $\diamond$

Of the Hamiltonian $\hat{H}$, we assume that molecules, when separated by a sufficient (still microscopic) distance, hardly interact. Since the details of the interaction term do not matter much in the end, let us focus for a moment on the part of $\hat{H}$ that does matter, the part we need to write down for calculating $n_{\text{eq},i}$. A key contribution is the kinetic energy of the center of mass of each molecule; another one the external field (e.g., electric, magnetic, or gravitational) to which each molecule is subject; another one the energy contributions of internal degrees of freedom (e.g., rotational, vibrational, or librational) of each molecule. We write $\hat{H}_{1i}$ for the 1-molecule Hamiltonian combining these contributions, $\hat{H}_{0i}$ for the second quantized version of $\hat{H}_{1i}$ (i.e., the operator on $\mathcal{F}_i$ acting like $\hat{H}_{1i}$ on each particle), and $\hat{H}_0$ for the combination of those over all types i ,

$$\hat{H}_0 := \sum_{i=1}^r \hat{I}_1 \otimes \cdots \otimes \hat{I}_{i-1} \otimes \hat{H}_{0i} \otimes \hat{I}_{i+1} \otimes \cdots \otimes \hat{I}_r \quad (19)$$

with $\hat{I}_i$ the identity on $\mathcal{F}_i$. Another key contribution to the full Hamiltonian $\hat{H}$ comes from the *rest energy* of each molecule; that is, apart from the relativistic contribution from the rest mass of the particles (which is irrelevant for chemical reactions because electron-positron or quark-antiquark pair creation do not occur), the *ground state energy* E_{0i} of each molecule. For example in the reaction (6), δE represents the binding energy between A and B within a C molecule, meaning that

$$E_{0C} = E_{0A} + E_{0B} - \delta E. \quad (20)$$

Likewise in the general case (14), the E_{0i} have to satisfy

$$\nu_{\ell 1} E_{01} + \cdots + \nu_{\ell r} E_{0r} = \tilde{\nu}_{\ell 1} E_{01} + \cdots + \tilde{\nu}_{\ell r} E_{0r} + \delta E_{\ell} \quad (21)$$

for every $\ell = 1, \dots, L$. Up to some remaining freedom, the E_{0i} can be determined from the known $\delta E_{\ell}, \nu_{\ell i}, \tilde{\nu}_{\ell i}$ by solving (21); if a solution to (21) did not exist, it would signal the existence of a circle of reactions from (14) that produce energy while returning the same number of each molecule, which is physically impossible. We will see in Remark 3 below that the freedom in the E_{0i} does not affect either $\hat{\rho}_{\text{gc}}$ or $n_{\text{eq},i}$. Suppose we know the E_{0i} ; we can then define

$$\hat{H}_* := \hat{H}_0 + \sum_{i=1}^r E_{0i} \hat{N}_i, \quad (22)$$

which is equivalent to adding E_{0i} to the 1-particle Hamiltonian $\hat{H}_{1i}$ before the second quantization.

Of the full Hamiltonian again,

$$\hat{H} = \hat{H}_* + \hat{V}, \quad (23)$$

we assume that the interaction term $\hat{V}$ is mostly negligibly small (namely, except during a chemical reaction) and contains non-zero transition elements corresponding to every reaction (14), but not for any transition that is not of the form (14). That is, we assume that the conserved quantities of (14) are the only macroscopic conserved observables. In detail, using (simple) tools from linear algebra, consider the r -dimensional real space $\mathcal{R}$ with axes labeled $n_1, \dots, n_r$, and let $\mathcal{L}$ be the subspace spanned by the L vectors $(\nu_{\ell 1} - \tilde{\nu}_{\ell 1}, \dots, \nu_{\ell r} - \tilde{\nu}_{\ell r})$. Any change in particle numbers due to reactions of the form (14) lies in $\mathcal{L}$, any conserved linear combination of $n_1, \dots, n_r$ is orthogonal to $\mathcal{L}$. (In fact, the deeper reason we allow real rather than integer components in $\mathcal{R}$ is that we allow real coefficients in these linear combinations.) Choose a complete set $F_1, \dots, F_{K-1}$ of conserved linear combinations with

$$K = \dim(\mathcal{L}^\perp) + 1 = r + 1 - \dim \mathcal{L} \quad (24)$$

(which is equal to $r + 1 - L$ if the L vectors just mentioned are linearly independent). That is, choose a linear mapping (a $(K - 1) \times r$ -matrix) $F : \mathcal{R} \rightarrow \mathbb{R}^{K-1}$ with kernel

$$F^{-1}(0) = \mathcal{L}. \quad (25)$$

By the dimension formula

$$\dim \text{kernel}(F) + \dim \text{image}(F) = r, \quad (26)$$

F has full rank, $\text{rank}(F) = \dim \text{image}(F) = K - 1$, and for every $k = 1, \dots, K - 1$, $F_k(n_1, \dots, n_r)$ is conserved during every reaction (14). (Put differently, the rows $F_1, \dots, F_{K-1}$ of the matrix F form a basis of $\mathcal{L}^\perp$.) As a consequence, the observables

$$\hat{Q}_k := F_k(\hat{N}_1, \dots, \hat{N}_r) \quad (27)$$

are conserved, i.e., they commute with $\hat{H}$. They also commute with each other because $\hat{N}_1, \dots, \hat{N}_r$ do. Any other conserved linear combinations of number operators are linear combinations of the $\hat{Q}_k$ because we assumed that the transitions allowed by $\hat{H}$ between different sectors $\mathcal{F}_1^{(n_1)} \otimes \dots \otimes \mathcal{F}_r^{(n_r)}$ are exactly those allowed by the reactions (14). We assume that there are no further conserved macroscopic observables.

Now set $\hat{Q}_K := \hat{H}$; consider the generalized micro-canonical subspace $\mathcal{H}_{\text{gmc}}$ as defined in (8) with $Q_k = F_k(n_{01}, \dots, n_{0r})$ (and suitably small ΔQ_k) for $k = 1, \dots, K - 1$ and $Q_K = E$, $\Delta Q_K = \Delta E$; consider further the generalized Gibbs density matrix $\hat{\rho}_{\text{gG}}$ as defined in (7) with the values of λ_k chosen to satisfy (10).

Remark 2. If we had chosen F differently, it would not have changed $\hat{\rho}_{\text{gG}}$. In contrast, if we had chosen F differently, it would have changed $\hat{\rho}_{\text{gmc}}$ (though presumably not in a very relevant way). We prove both statements in Appendix A. $\diamond$

Now we apply the general Gibbs principle of Section 1. We obtain that there is a K -parameter family of thermal equilibrium states. (For example in (6), there is a 3-parameter family of thermal equilibrium states; the three parameters can be taken to

be the energy (or, for that matter, temperature), $n_A - n_B$, and $n_A + n_C$.) The thermal equilibrium states can be represented by the generalized Gibbs density matrix

$$\hat{\rho}_{\text{gG}} = Z_{\text{gG}}^{-1} \exp \left(\sum_{k=1}^{K-1} \lambda_k \hat{Q}_k + \lambda_K \hat{H} \right) \quad (28)$$

with real parameters $\lambda_1, \dots, \lambda_K$. We write $-\beta$ for λ_K ; since $\hat{H}$ is bounded from below and unbounded, λ_K must be negative and thus β positive. Since $\hat{H} = \hat{H}_* + \hat{V}$ with $\hat{V}$ small, we can replace $\hat{H}$ by $\hat{H}_*$,

$$\hat{\rho}_{\text{gG}} \approx Z_{\text{gG}}^{-1} \exp \left(\sum_{k=1}^{K-1} \lambda_k \hat{Q}_k - \beta \hat{H}_* \right). \quad (29)$$

Since $\hat{Q}_k = F_k(\hat{N}_1, \dots, \hat{N}_r)$ and F_k is a linear function

$$F_k(n_1, \dots, n_r) = \sum_{i=1}^r F_{ki} n_i, \quad (30)$$

we can write $\hat{Q}_k = \sum_{i=1}^r F_{ki} \hat{N}_i$ and

$$\hat{\rho}_{\text{gG}} \approx Z_{\text{gG}}^{-1} \exp \left(-\beta (\hat{H}_* - \sum_{i=1}^r \mu_{*i} \hat{N}_i) \right) \quad (31)$$

with

$$\mu_{*i} = \beta^{-1} \sum_{k=1}^{K-1} \lambda_k F_{ki}. \quad (32)$$

By (22),

$$\hat{\rho}_{\text{gG}} \approx \hat{\rho}_{\text{gc}} = Z_{\text{gc}}^{-1} \exp \left(-\beta (\hat{H}_0 - \sum_{i=1}^r \mu_{0i} \hat{N}_i) \right) \quad (33)$$

with $Z_{\text{gc}} = Z_{\text{gG}}$ and

$$\mu_{0i} = \mu_{*i} - E_{0i}. \quad (34)$$

The right-hand side of (33) is exactly what is meant by the formula (1c) for the grand-canonical density matrix $\hat{\rho}_{\text{gc}}$ that arises here as a special case of $\hat{\rho}_{\text{gG}}$. The $r+1$ coefficients $\mu_{01}, \dots, \mu_{0r}, \beta$ are determined by the K conditions (10) together with the L conditions

$$\sum_{i=1}^r (\mu_{0i} + E_{0i}) (\nu_{\ell i} - \tilde{\nu}_{\ell i}) = 0, \quad (35)$$

which follow from $F^{-1}(0) \supseteq \mathcal{L}$ (and of which $\dim \mathcal{L}$ many are independent). By (19), (33) can be rewritten as

$$\hat{\rho}_{\text{gc}} = \bigotimes_{i=1}^r \hat{\rho}_i := \bigotimes_{i=1}^r Z_i^{-1} \exp(-\beta (\hat{H}_{0i} - \mu_{0i} \hat{N}_i)). \quad (36)$$

If we write $\hat{H}_{1i}$ for the 1-particle Hamiltonian whose second quantization is $\hat{H}_{0i}$, then each tensor factor in (36) is a canonical density matrix with $\hat{H}_{0i}$ replaced by the second quantization of $\hat{H}_{1i} - \mu_{0i}\hat{I}$. This fact also provides a direct interpretation of the physical meaning of μ_{0i} : The thermal density matrix looks as if it were canonical and molecule i had ground state energy $-\mu_{0i}$.

Finally, the desired numbers $n_{\text{eq},i}$ characterizing the chemical equilibrium are then given by

$$n_{\text{eq},i} = \text{tr}(\hat{\rho}_{\text{gmc}}\hat{N}_i) \quad (37a)$$

$$\approx \text{tr}(\hat{\rho}_{\text{gc}}\hat{N}_i) \quad (37b)$$

$$= \text{tr}_{\mathcal{F}_i}(\hat{\rho}_i\hat{N}_i) = \frac{\text{tr}(\hat{N}_i \exp(-\beta(\hat{H}_{0i} - \mu_{0i}\hat{N}_i)))}{\text{tr} \exp(-\beta(\hat{H}_{0i} - \mu_{0i}\hat{N}_i))} \quad (37c)$$

$$= \frac{1}{\beta} \frac{\partial}{\partial \mu_{0i}} \log Z_{\text{gc}}(\beta, \mu_{01}, \dots, \mu_{0r}) \quad (37d)$$

using (19); the function $-(1/\beta) \log Z_{\text{gc}}(\beta, \mu_{01}, \dots, \mu_{0r})$ is known as the *grand potential* (e.g., [1, (5.73)], [44, (2.7.13)]). Note that, while (37c) is an expression that one might have guessed right from the start, our derivation has achieved two things: First, provided reasons for why (37) is true, and second, provided a way of computing the μ_{0i} from the known quantities $n_{0i}, \delta E_\ell$ by means of (35) and (10).

Remark 3. Different values of E_{0i} solving (21) would lead to the same $\hat{\rho}_{\text{gG}} \approx \hat{\rho}_{\text{gc}}$ (neglecting $\hat{V}$) and the same $n_{\text{eq},i}$; they also lead to the same $\hat{\rho}_{\text{gmc}}$, provided $\Delta Q_k = 0$ and Q_k is an eigenvalue of $\hat{Q}_k$ for $k = 1, \dots, K-1$.² We prove this in Appendix B. $\diamond$

In the example of (6), E_{0A} and E_{0B} can be chosen arbitrarily, E_{0C} is determined by (20), (35) reduces to $\mu_{0C} = \mu_{0A} + \mu_{0B} + \delta E$, and (10) reduces to the three conditions (with $\hat{\rho}_A$ etc. as in (36))

$$\text{tr}(\hat{\rho}_A\hat{N}_A) - \text{tr}(\hat{\rho}_B\hat{N}_B) = n_{0A} - n_{0B} \quad (38a)$$

$$\text{tr}(\hat{\rho}_A\hat{N}_A) + \text{tr}(\hat{\rho}_C\hat{N}_C) = n_{0A} + n_{0C} \quad (38b)$$

$$\sum_{i=A,B,C} \left[\text{tr}(\hat{\rho}_i\hat{H}_{0i}) + E_{0i} \text{tr}(\hat{\rho}_i\hat{N}_i) \right] = E, \quad (38c)$$

which together determine μ_{0A}, μ_{0B} , and β . (Note that E would change if we changed E_{0A}, E_{0B} , see Remark 3.)

Remark 4. The reaction rates depend on $\hat{V}$, but the equilibrium state and the $n_{\text{eq},i}$ do not, as long as $\hat{V}$ is small. Related questions for non-small $\hat{V}$ have been studied in [7, 4]. $\diamond$

²Otherwise, $\hat{\rho}_{\text{gmc}}$ still stays *approximately* the same, provided the density of states of $\hat{Q}_k$ is a quickly increasing function, so most eigenvectors have eigenvalue near the right end of $[Q_k - \Delta Q_k, Q_k]$.

3 Main Claims

We now present our main statements. Apart from Statement 1b, the derivations of the statements are given below in the following sections. Let $\Lambda \subset \mathbb{R}^3$ denote the available volume of the quantum system considered and

$$\bar{S} := \Lambda \setminus S \quad (39)$$

the spatial complement of a subset S (*not* the closure of a set). We take $\hat{\rho}_{\text{gmc}}$ as defined in (9) and $\hat{\rho}_{\text{gG}}$ as defined in (7). For extensive $\hat{Q}_k$ as in (13), it follows that

$$\hat{\rho}_{\text{gG}} \approx \hat{\rho}_{\text{gG}}^S \otimes \hat{\rho}_{\text{gG}}^{\bar{S}} \quad (40)$$

with $\hat{\rho}_{\text{gG}}^S$ formed according to (7) from the $\hat{Q}_k^S$ and likewise for $\bar{S}$. This also entails that

$$\text{tr}^{\bar{S}} \hat{\rho}_{\text{gG}} \approx \hat{\rho}_{\text{gG}}^S. \quad (41)$$

Statement 1a. (Generalized Gibbs Density Matrix) *Let Λ be a subset of $\mathbb{R}^3$, $\mathcal{H} = \mathcal{H}^\Lambda$ a Hilbert space, and for every $S \subseteq \Lambda$ let $\mathcal{H}^S$ be a Hilbert space such that for $S_1 \subseteq S_2 \subseteq \Lambda$, $\mathcal{H}^{S_2}$ factorizes into $\mathcal{H}^{S_2} = \mathcal{H}^{S_1} \otimes \mathcal{H}^{S_2 \setminus S_1}$. Suppose the self-adjoint operators $\hat{Q}_1, \dots, \hat{Q}_K$ on $\mathcal{H}$ are bounded from below and commute with each other, and that each is (approximately) extensive as in (13). Then for $\lambda_1, \dots, \lambda_K$ satisfying (10), large $\dim \mathcal{H}_{\text{gmc}}$, and small $S \subset \Lambda$,*

$$\text{tr}^{\bar{S}} \hat{\rho}_{\text{gmc}} \approx \hat{\rho}_{\text{gG}}^S. \quad (42)$$

In particular, by (41), (42) entails that $\hat{\rho}_{\text{gmc}}$ and $\hat{\rho}_{\text{gG}}$ are S -equivalent, and thus that $\hat{\rho}_{\text{gmc}}$ and $\hat{\rho}_{\text{gG}}$ are locally equivalent.

We give a derivation in Section 5.

Statement 1b. (Grand-Canonical Density Matrix) *Let $\mathcal{H} = \mathcal{F}_1 \otimes \dots \otimes \mathcal{F}_r$ with $\mathcal{F}_i$ the bosonic or fermionic Fock space over the 1-particle space $\mathcal{H}_{1i}$ and $\Lambda \subset \mathbb{R}^3$. Suppose*

$$\hat{H} \approx \hat{H}_* = \hat{H}_0 + \sum_{i=1}^r E_{0i} \hat{N}_i \quad (43)$$

with $\hat{H}_0$ as in (19) and $\hat{H}_{0i}$ the second quantization of a 1-particle Hamiltonian $\hat{H}_{1i}$ that is bounded from below. Suppose for every $S \subseteq \Lambda$,

$$\mathcal{H}_{1i} = \mathcal{H}_{1i}^S \oplus \mathcal{H}_{1i}^{\bar{S}} \quad (44)$$

and

$$\hat{H}_{1i} \approx \hat{H}_{1i}^S \oplus \hat{H}_{1i}^{\bar{S}}. \quad (45)$$

Suppose (14) for $\ell = 1, \dots, L$ are the (only) possible reactions (i.e., changes in particle numbers), and (21) holds. Choose any F satisfying (25), and define $\hat{Q}_k$

by (27) (so that $[\hat{H}, \hat{Q}_k] = 0$) and $\hat{Q}_K = \hat{H}$. Then for $\dim \mathcal{H}_{\text{gmc}} \gg 1$ and μ_{0i} satisfying (10) and (35),

$$\hat{\rho}_{\text{gc}} := Z_{\text{gc}}^{-1} \exp\left(-\beta(\hat{H}_0 - \sum_i \mu_{0i} \hat{N}_i)\right) \quad (46)$$

is locally equivalent to $\hat{\rho}_{\text{gmc}}$.

Statement 1b follows from 1a through the reasoning of Section 2. The condition (45) is actually satisfied for reasonable 1-particle Hamiltonians, as we argue in Section 4.3 for the Laplacian.

Statement 2a. (Ensemble Typicality) *In the setting of Statement 1a, most pure states $\Psi \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$ are such that the reduced density matrix of a small region $S \subset \Lambda$ is approximately a generalized Gibbs density matrix:*

$$\hat{\rho}_{\Psi}^S := \text{tr}^{\bar{S}} |\Psi\rangle\langle\Psi| \approx \hat{\rho}_{\text{gG}}^S. \quad (47)$$

Statement 2b. (Grand-Canonical Typicality) *In the setting of Statement 1b, most pure states $\Psi \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$ are such that the reduced density matrix of a small region $S \subset \Lambda$ is approximately grand-canonical:*

$$\hat{\rho}_{\Psi}^S = \text{tr}^{\bar{S}} |\Psi\rangle\langle\Psi| \approx \hat{\rho}_{\text{gc}}^S. \quad (48)$$

For the derivation, an application of a theorem of [36], see Section 6. “Most” refers to the uniform measure over $\mathbb{S}(\mathcal{H}_{\text{gmc}})$.

For the next statement, we need the notion of conditional wave function ψ^S , which we briefly explain now (for a detailed discussion see Section 7.1 and the cited references therein). The concept starts from the wave function Ψ of S and B together and makes use of an orthonormal basis (ONB) $b = \{|b_1\rangle, |b_2\rangle, \dots\}$ of $\mathcal{H}^B$ (or generalized ONB, such as the position basis); the conditional wave function is the random wave function

$$\psi^S = \mathcal{N} \langle b_J | \Psi \rangle_B \in \mathbb{S}(\mathcal{H}^S), \quad (49)$$

where $\mathcal{N}$ is the normalizing factor, $\langle \cdot | \cdot \rangle_B$ is the partial inner product, and the basis vector b_J is chosen randomly with Born distribution,

$$\mathbb{P}(J = j) = \|\langle b_j | \Psi \rangle_B\|_S^2. \quad (50)$$

The conditional wave function can be thought of as what the collapsed wave function of S would be after an ideal quantum measurement of the basis b on B [17, Footnote 2].

In the following, the GAP measures play a role. For every density matrix $\hat{\rho}$ on a Hilbert space $\mathcal{H}$, the measure $\text{GAP}_{\hat{\rho}}$ is a probability measure on the unit sphere of $\mathcal{H}$ whose associated density matrix is $\hat{\rho}$; it is the most spread-out measure for the given density matrix $\hat{\rho}$; see Section 7.1 for the definition.

We now answer the question, raised in the introduction, of what $\mathbb{P}_{\text{gc}}$ is, the probability distribution of the wave function corresponding to the grand-canonical ensemble.

We answer it by providing the typical distribution of the conditional wave function ψ^S . The answer is twofold, as it depends on how the basis b is chosen. In general, ψ^S (and its distribution) depends on the choice of b , and while b can be chosen arbitrarily, one is often particularly interested in taking b the position (or configuration) basis [5]. We provide two results assuming that S is a small spatial region and $B = \bar{S}$: one result in which b is a *typical* (i.e., random) ONB, and one in which b is *typical among those that diagonalize the conserved operators* $\hat{Q}_k^{\bar{S}}$ (respectively, the particle number operators $\hat{N}_i^{\bar{S}}$). The first result (Statement 3) applies whenever b is unrelated to the joint eigenbasis of $\hat{H}^{\bar{S}}$ and the $\hat{Q}_k^{\bar{S}}$ (respectively, $\hat{N}_i^{\bar{S}}$); the second (Statements 4a and 4b) whenever there is no simple relation between b and $\hat{H}^{\bar{S}}$ other than that both b and a suitable eigenbasis of $\hat{H}^{\bar{S}}$ diagonalize the $\hat{Q}_k^{\bar{S}}$ (the $\hat{N}_i^{\bar{S}}$)—this seems like a reasonable approximation for the position basis.

For any random variable X , let $\mathcal{L}_X$ (“law of X ”) denote its probability distribution.

Statement 3. ($\mathbb{P}_{\text{gG}}$ and $\mathbb{P}_{\text{gc}}$ for Typical ONB) *In the setting of Statement 1a (or 1b) with S a small spatial region, for most $\Psi \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$ and most ONBs b of $\mathcal{H}^{\bar{S}}$, the conditional wave function (49) has distribution*

$$\mathcal{L}_{\psi^S} \approx \text{GAP}_{\hat{\rho}_{\text{gG}}^S} \quad (51)$$

(respectively, $\approx \text{GAP}_{\hat{\rho}_{\text{gc}}^S}$).

For the derivation, an application of a theorem of [17], see Section 7.2.

In the following, we use the notation

$$\mu = \bigoplus_j p(j) \mu_j \quad (52)$$

for the probability distribution that is the mixture of the probability distributions μ_j with weights $p(j) \geq 0$, $\sum_j p(j) = 1$. Equivalently, if $\mathcal{L}_{X_j} = \mu_j$ and $\mathbb{P}(J = j) = p(j)$, then $\mathcal{L}_{X_J} = \mu$. We also use the notation

$$\hat{P}(\hat{A} = a) \quad (53)$$

for the projection to the eigenspace of $\hat{A}$ with eigenvalue a and

$$\hat{P}(\hat{A}_1 = a_1, \dots, \hat{A}_r = a_r) \quad (54)$$

for the projection to the joint eigenspace of commuting $\hat{A}_1, \dots, \hat{A}_r$. By the Born rule, the joint probability distribution of the outcomes in a simultaneous quantum measurement of the observables $\hat{A}_1, \dots, \hat{A}_r$ on a system with density matrix $\hat{\rho}$ is given by

$$\mathbb{P}(\hat{A}_1 = a_1, \dots, \hat{A}_r = a_r) = \text{tr} \left[\hat{\rho} \hat{P}(\hat{A}_1 = a_1, \dots, \hat{A}_r = a_r) \right]. \quad (55)$$

Statement 4a. ($\mathbb{P}_{\text{gG}}$ for ONB Diagonalizing $\hat{Q}_k^{\bar{S}}$) In the setting of Statement 1a, suppose that $S \subset \Lambda$ is a small region and that for every $k = 1, \dots, K-1$, $\Delta Q_k = 0$ and Q_k is an eigenvalue of $\hat{Q}_k$. Then for most $\Psi \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$ and most ONBs b of $\mathcal{H}^{\bar{S}}$ that diagonalize $\hat{Q}_1^{\bar{S}}, \dots, \hat{Q}_{K-1}^{\bar{S}}$ (but not $\hat{Q}_K^{\bar{S}} = \hat{H}^{\bar{S}}$),

$$\mathcal{L}_{\psi S} \approx \mathbb{P}_{\text{gG}} := \bigoplus_{q_1^S, \dots, q_{K-1}^S} p(q_1^S, \dots, q_{K-1}^S) \text{ GAP}_{\hat{\rho}^S(q_1^S, \dots, q_{K-1}^S)}, \quad (56)$$

where

$$p(q_1^S, \dots, q_{K-1}^S) = \text{tr}(\hat{\rho}_{\text{gG}}^S \hat{P}) \quad \text{with} \quad \hat{P} := \hat{P}(\hat{Q}_1^S = q_1^S, \dots, \hat{Q}_{K-1}^S = q_{K-1}^S) \quad (57)$$

and

$$\hat{\rho}^S(q_1^S, \dots, q_{K-1}^S) = \frac{1}{p(q_1^S, \dots, q_{K-1}^S)} \hat{P} \hat{\rho}_{\text{gG}}^S \hat{P}. \quad (58)$$

Statement 4b. ($\mathbb{P}_{\text{gc}}$ for ONB Diagonalizing $\hat{N}_i^{\bar{S}}$) In the setting of Statement 1b, suppose that $S \subset \Lambda$ is a small region and that for every $k = 1, \dots, K-1$, $\Delta Q_k = 0$ and Q_k is an eigenvalue of $\hat{Q}_k$. Then for most $\Psi \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$ and most ONBs b of $\mathcal{H}^{\bar{S}}$ that diagonalize $\hat{N}_1^{\bar{S}}, \dots, \hat{N}_r^{\bar{S}}$,

$$\mathcal{L}_{\psi S} \approx \mathbb{P}_{\text{gc}} := \bigoplus_{n_1^{\bar{S}}, \dots, n_r^{\bar{S}}} p_n(n_1^{\bar{S}}, \dots, n_r^{\bar{S}}) \text{ GAP}_{\hat{\rho}(n_1^{\bar{S}}, \dots, n_r^{\bar{S}})}, \quad (59)$$

where

$$p_n(n_1^{\bar{S}}, \dots, n_r^{\bar{S}}) = \text{tr}(\hat{\rho}_{\text{gmc}} \hat{P}_n) \quad \text{with} \quad \hat{P}_n := \hat{P}(\hat{N}_1^{\bar{S}} = n_1^{\bar{S}}, \dots, \hat{N}_r^{\bar{S}} = n_r^{\bar{S}}) \quad (60)$$

and

$$\hat{\rho}(n_1^{\bar{S}}, \dots, n_r^{\bar{S}}) = \frac{1}{p_n(n_1^{\bar{S}}, \dots, n_r^{\bar{S}})} \text{tr}^{\bar{S}}[\hat{P}_n \hat{\rho}_{\text{gmc}} \hat{P}_n]. \quad (61)$$

Remark 5. If the general Gibbs principle is more generally valid than under the assumptions of Statement 1a (which is plausible as pointed out in Section 4.2), then the expression for $\mathbb{P}_{\text{gc}}$ can be simplified further:

$$\mathbb{P}_{\text{gc}} \approx \bigoplus_{q_1^S, \dots, q_{K-1}^S} p(q_1^S, \dots, q_{K-1}^S) \text{ GAP}_{\hat{\rho}^S(q_1^S, \dots, q_{K-1}^S)}, \quad (62)$$

where

$$p(q_1^S, \dots, q_{K-1}^S) = \text{tr}(\hat{\rho}_{\text{gc}}^S \hat{P}) \quad \text{with} \quad \hat{P} \text{ as in (57)} \quad (63)$$

and

$$\hat{\rho}^S(q_1^S, \dots, q_{K-1}^S) = \frac{1}{p(q_1^S, \dots, q_{K-1}^S)} \hat{P} \hat{\rho}_{\text{gc}}^S \hat{P}. \quad (64)$$

◇

Statement 4b is actually not a special case of Statement 4a because only certain combinations of $\hat{N}_i$ are conserved as the $\hat{Q}_k$, and while in Statement 4a we considered bases diagonalizing the $\hat{Q}_k^{\bar{S}}$ (i.e., certain combinations of the $\hat{N}_i^{\bar{S}}$), we consider in Statement 4b bases diagonalizing *all* $\hat{N}_i^{\bar{S}}$. That is because we are interested in the position/configuration basis, which diagonalizes all $\hat{N}_i^{\bar{S}}$; on the other hand, Statement 4a is the simpler statement, and can be applicable to general $\hat{Q}_k$ that are not related to number operators.

We also note in passing that while the $\oplus$ symbol for measures means merely, according to its definition (52), the mixture of several measures, something more is true in (56) and (62): the measures are even disjoint and, on top of that, their supports even lie in mutually orthogonal subspaces.

The next statement concerns the approach (time evolution) towards thermal equilibrium. As many earlier works such as [57, 37, 30, 15], we take “approach” to mean that for most $t \geq 0$ in the long run, the system is in thermal equilibrium. And we take “thermal equilibrium” to mean that $\hat{\rho}_{\Psi_t}^S \approx \hat{\rho}_{\text{gG}}^S$ and $\mathcal{L}_{\psi^S} \approx \mathbb{P}_{\text{gG}}$.

Statement 5. (Approach to Equilibrium) *Consider the setting of Statement 3 (or 4a or 4b) with small spatial region $S \subset \Lambda$. Suppose $\hat{H}$ satisfies the eigenstate thermalization hypothesis (ETH): for eigenvectors $\phi_1, \phi_2 \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$ of $\hat{H}$ that belong to different eigenspaces of $\hat{H}$,*

$$\text{tr}^{\bar{S}} |\phi_1\rangle\langle\phi_1| \approx \text{tr}^{\bar{S}} \hat{\rho}_{\text{gmc}} \quad (65a)$$

$$\text{tr}^{\bar{S}} |\phi_1\rangle\langle\phi_2| \approx 0. \quad (65b)$$

Then for every $\Psi_0 \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$ for most $t \geq 0$, the reduced density matrix of $\Psi_t = e^{-i\hat{H}t}\Psi_0$ is

$$\hat{\rho}_{\Psi_t}^S = \text{tr}^{\bar{S}} |\Psi_t\rangle\langle\Psi_t| \approx \hat{\rho}_{\text{gG}}^S \quad (\text{respectively, } \hat{\rho}_{\text{gc}}^S). \quad (66)$$

Furthermore, for every $\Psi_0 \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$ for most ONBs b as in Statement 3 (respectively, 4a or 4b) for most $t \geq 0$, the conditional wave function $\psi^S(t)$ obtained from Ψ_t is (approximately) distributed as in (51) (respectively, (56) or (59)).

The version of ETH expressed in (65a)-(65b), due to Srednicki [46], is the one appropriate for *microscopic* thermal equilibrium (“MITE”) [14]; for macroscopic thermal equilibrium, a different condition would be relevant [15, 14, 43].

4 Discussion

4.1 Comparison to Maximum Entropy Principle

The density matrices $\hat{\rho}_{\text{can}}$ and $\hat{\rho}_{\text{gc}}$ are often introduced in the literature as the maximizers of the von Neumann entropy S_{vN} (5) under the constraint $\text{tr}(\hat{\rho}\hat{H}) = E$ (and, if appropriate, $\text{tr}(\hat{\rho}\hat{N}) = n$) (e.g., [1, 12, 26], classically [24]). While it is mathematically

correct that they *are* these maximizers, a derivation based merely on this fact is considerably weaker than the one we have presented, and in fact rather questionable, for at least two reasons.

First, the maximization problem leads to a representation of *subjective* probability (or the knowledge of an observer), but if statistical mechanics were limited to subjective probability then it would not be justified in most applications; in particular, it could not treat any events that take place in the absence of observers (e.g., the formation of stars before humans even existed). In contrast, there is nothing subjective about $\text{tr}^{\bar{S}} |\Psi\rangle\langle\Psi|$; that is, we have shown how $\hat{\rho}_{\text{gc}}$ actually occurs in nature.

Second, it remains unclear why one should constrain the *expectation value* of a probability distribution or density matrix, even when determining the subjective probability distribution of an observer with limited information. After all, if a person was looking for their car and somehow knew only that its location has latitude 50° N, then the subjective probability distribution would be concentrated on the circle of latitude 50° N, rather than including other latitudes in such a fashion that the *expected* latitude is 50° N. Therefore, even for subjective probability, $\hat{\rho}_{\text{mc}}$ or $\hat{\rho}_{\text{gmc}}$ would be much more relevant; it is only after realizing and using the equivalence of ensembles that they can be replaced by $\hat{\rho}_{\text{can}}$ or $\hat{\rho}_{\text{gc}}$. A precise version of this equivalence is provided by our Statements 2a and 2b.

Remark 6. The second issue above was mentioned by Balian [1, Sec. 4.1.2], who suggested that prescribing the expectation value of an observable $\hat{A}$ made sense when considering *subsystems*, of which there are many, and each may have a different value of $\hat{A}$. However, that seems like mixing up the description and the justification of $\hat{\rho}_{\text{can}}$. If, as Balian’s reasoning suggests, $\hat{\rho}_{\text{can}}$ can only apply to subsystems S , while only $\hat{\rho}_{\text{mc}}$ can apply to full systems, then $\hat{\rho}_{\text{can}}^S$ can only be justified as $\text{tr}^{\bar{S}} \hat{\rho}_{\text{mc}}$, and the maximizer of S_{VN} for S (under whichever constraints) would be irrelevant unless it agreed with $\text{tr}^{\bar{S}} \hat{\rho}_{\text{mc}}$. That is, the reasoning apparently undercuts the use of S_{VN} for justifying $\hat{\rho}_{\text{can}}$. For us, the consideration of subsystems also plays an important role, for example through the concept of local equivalence of density matrices, but the logic is different in our case, as we do not use subjective probability. $\diamond$

Another question that arises in this context is whether $\hat{\rho}_{\text{mc}}$ (or $u_{\mathbb{S}(\mathcal{H}_{\text{mc}})}$) itself has the status of subjective probability, given that it simply assigns equal weight to states with energies in $[E - \Delta E, E]$. Our answer is: no; rather, it is a characteristic property of *thermal equilibrium* that the micro-state (here, Ψ) behaves like the overwhelming majority of micro-states with the same values of E (and, if appropriate, $Q_1, \dots, Q_{K-1}$); a Ψ in thermal equilibrium should for this reason be typical relative to the measure $u_{\mathbb{S}(\mathcal{H}_{\text{mc}})}$ (respectively, $u_{\mathbb{S}(\mathcal{H}_{\text{gmc}})}$), whose density matrix is $\hat{\rho}_{\text{mc}}$ ($\hat{\rho}_{\text{gmc}}$).

4.2 Plausibility of the General Gibbs Principle

“Equivalence of ensembles” means that one thermodynamic ensemble can be replaced, in either classical or quantum statistical mechanics, by another; many variations of this theme are known, corresponding to different senses of “equivalence.” We now describe a heuristic consideration that makes it plausible that $\hat{\rho}_{\text{gmc}}$ as in (9) is equivalent to $\hat{\rho}_{\text{gG}}$

as in (7), without referring to a precise sense of equivalence. (A similar consideration applies already to $\hat{\rho}_{\text{mc}}$ and $\hat{\rho}_{\text{can}}$.)

Any ONB $\{\phi_j\}$ that jointly diagonalizes $\hat{Q}_1, \dots, \hat{Q}_K$ also diagonalizes $\hat{\rho}_{\text{gmc}}$ and $\hat{\rho}_{\text{gG}}$, so the relevant question is whether their *eigenvalues* “look similar.” Each of the two density matrices defines a Born distribution in the real space spanned by K axes labeled with $q_1, \dots, q_K$, given by

$$p_\alpha(q_1, \dots, q_K) = \text{tr}(\hat{\rho}_\alpha \hat{P}(\hat{Q}_1 = q_1, \dots, \hat{Q}_K = q_K)) \quad (67)$$

with $\alpha = \text{gmc}$ or $\alpha = \text{gG}$, and the consideration aims to show that the two probability distributions “look similar” by showing that both are sharply peaked around the point $(Q_1, \dots, Q_K)$: p_{gmc} because it is concentrated in the rectangle $\prod_k [Q_k - \Delta Q_k, Q_k]$ and ΔQ_k is small, and p_{gG} because its expectation is $(Q_1, \dots, Q_K)$ by (10), much larger values of q_k are suppressed by the exponential dependence in (7) (provided $\lambda_k < 0$), and much smaller values are suppressed provided the joint “density of states” of $\hat{Q}_1, \dots, \hat{Q}_K$ (i.e., the dimension of the spectral subspace associated with a cube around $(q_1, \dots, q_K)$ with side length ΔQ that is small on the macroscopic scale, divided by the volume $(\Delta Q)^K$ of the cube and then approximated by a smooth function of $q_1, \dots, q_K$) increases quickly with each of the q_k variables, as it would be the case for relevant examples of macroscopic observables such as energy or particle number.

It is possible to make this consideration a little bit sharper: A relevant sense of “equivalence” could be that

$$\text{for macroscopic observables } \hat{A}, \quad \text{tr}(\hat{\rho}_{\text{gmc}} \hat{A}) \approx \text{tr}(\hat{\rho}_{\text{gG}} \hat{A}). \quad (68)$$

The width of the peak will be different for p_{gmc} and p_{gG} :

Example 1. In the canonical case $K = 1$, $\hat{Q}_1 = \hat{H}$, $\hat{\rho}_{\text{gmc}} = \hat{\rho}_{\text{mc}}$, and $\hat{\rho}_{\text{gG}} = \hat{\rho}_{\text{can}}$, the density of states of $\hat{H} = -\Delta$ is a power law $f(q_1) \propto q_1^M$ with a large exponent M proportional to the particle number, and one finds that $p_{\text{gmc}}(q_1)f(q_1)$ has spread of order Q_1/M (see Appendix C), while $p_{\text{gG}}(q_1)f(q_1)$ has spread of order $Q_1/\sqrt{M}$, which is larger by the large factor $\sqrt{M}$. $\diamond$

To be sure, there are observables, such as

$$\mathbb{1}_{[-1/\sqrt{M}, -1/M] \cup [1/M, 1/\sqrt{M}]}(\hat{Q}_1/Q_1 - \hat{I}), \quad (69)$$

that yield ≈ 0 for the narrower peak but ≈ 1 for the wider peak; however, relevant macroscopic observables $\hat{A}$ should be insensitive to the width of the peak, which supports (68).

4.3 Laplacian on the Union of Regions

Consider two spatial regions $\Lambda_1, \Lambda_2 \subset \mathbb{R}^3$ bordering on each other along some surface Σ . We argue that the free 1-particle Hamiltonian associated with $\Lambda = \Lambda_1 \cup \Lambda_2$ is approximately, though not exactly, block diagonal with respect to the corresponding splitting $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ of the 1-particle Hilbert space, provided the surface Σ is “not

too large" (say, the volume of an ε -neighborhood of Σ in Λ for $\varepsilon \ll 1$ is small compared to the volumes of Λ_1 and Λ_2).

The argument focuses on the negative Laplacian as an example of a free Hamiltonian $\hat{H}_0$. If $\hat{H}_0$ were exactly block diagonal, then a wave function initial concentrated in Λ_1 would never enter Λ_2 , but it does. Here is another way of looking at the issue: the negative Laplacian in a region Λ becomes a self-adjoint operator only if we introduce boundary conditions on the boundary $\partial\Lambda$ of Λ ; suppose we always use Dirichlet boundary conditions (i.e., $\psi|_{\partial\Lambda} = 0$) to define the self-adjoint operator Δ_Λ ; then it is clear that $(-\Delta_{\Lambda_1}) \oplus (-\Delta_{\Lambda_2})$ (which requires ψ to vanish on Σ) is different from $-\Delta_\Lambda$ (which does not require ψ to vanish on Σ). Now the argument for being approximately block diagonal, i.e.,

$$-\Delta_\Lambda \approx (-\Delta_{\Lambda_1}) \oplus (-\Delta_{\Lambda_2}), \quad (70)$$

considers the discrete Laplacian (for simplicity in 1d) on the lattice $\varepsilon\mathbb{Z}$ with mesh width $\varepsilon > 0$ and (for simplicity) $\Lambda_1 = \{x \in \varepsilon\mathbb{Z} : x \leq 0\}$ and $\Lambda_2 = \{x \in \varepsilon\mathbb{Z} : x > 0\}$; then it notes that the difference between $-\Delta_\Lambda$ and $(-\Delta_{\Lambda_1}) \oplus (-\Delta_{\Lambda_2})$, i.e., between

$$\frac{1}{\varepsilon^2} \left(\begin{array}{ccc|ccc} \ddots & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ \hline & & & -1 & 2 & -1 \\ & & & -1 & 2 & -1 \\ & & & & -1 & \ddots \end{array} \right) \text{ and } \frac{1}{\varepsilon^2} \left(\begin{array}{ccc|ccc} \ddots & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & & & \\ \hline & & & 2 & -1 & \\ & & & -1 & 2 & -1 \\ & & & & -1 & \ddots \end{array} \right) \quad (71)$$

consists of just two entries—very little.

5 Derivation of Statement 1a: Generalized Gibbs Density Matrix

This derivation has parallels with considerations in [44, 28, 6, 22, 18]. However, we do not assume here that relations known from thermodynamics are valid.

For the purposes of this derivation, we pretend that the approximate equalities in (13) (and thus also (40) and (41)) are exact equalities. For any $S \subset \Lambda$, it follows that

$$0 = [\hat{Q}_k, \hat{Q}_{k'}] \quad (72a)$$

$$= [\hat{Q}_k^S \otimes \hat{I}^{\bar{S}} + \hat{I}^S \otimes \hat{Q}_k^{\bar{S}}, \hat{Q}_{k'}^S \otimes \hat{I}^{\bar{S}} + \hat{I}^S \otimes \hat{Q}_{k'}^{\bar{S}}] \quad (72b)$$

$$= [\hat{Q}_k^S, \hat{Q}_{k'}^S] \otimes \hat{I}^{\bar{S}} + \hat{I}^S \otimes [\hat{Q}_k^{\bar{S}}, \hat{Q}_{k'}^{\bar{S}}], \quad (72c)$$

so

$$[\hat{Q}_k^S, \hat{Q}_{k'}^S] = 0 = [\hat{Q}_k^{\bar{S}}, \hat{Q}_{k'}^{\bar{S}}]. \quad (73)$$

For $X = S, \bar{S}$ let $\{\phi_j^X : j \in \mathcal{J}^X\}$ be an ONB of $\mathcal{H}^X$ that is a joint eigenbasis of all $\hat{Q}_k^X$, and let q_{kj}^X be the corresponding eigenvalue. With the notation $\mathcal{J} := \mathcal{J}^S \times \mathcal{J}^{\bar{S}}$ and

$\phi_{jj'} := \phi_j^S \otimes \phi_{j'}^{\bar{S}}$, it follows that $\{\phi_{jj'} : (j, j') \in \mathcal{J}\}$ is an ONB of $\mathcal{H}$ that diagonalizes (among others) $\hat{Q}_1, \dots, \hat{Q}_K$. Let

$$\mathcal{J}_{\text{gmc}} := \left\{ (j, j') \in \mathcal{J} : \forall k : \hat{Q}_k \phi_{jj'} = q_k \phi_{jj'} \text{ with } q_k \in [Q_k - \Delta Q_k, Q_k] \right\} \quad (74a)$$

$$= \left\{ (j, j') \in \mathcal{J} : \forall k : q_{kj}^S + q_{kj'}^{\bar{S}} \in [Q_k - \Delta Q_k, Q_k] \right\}, \quad (74b)$$

so $\text{span}\{\phi_{jj'} : (j, j') \in \mathcal{J}_{\text{gmc}}\} = \mathcal{H}_{\text{gmc}}$. Thus, writing $d_{\text{gmc}} := \dim \mathcal{H}_{\text{gmc}}$,

$$\hat{\rho}_{\text{gmc}} = \frac{1}{d_{\text{gmc}}} \sum_{(j, j') \in \mathcal{J}_{\text{gmc}}} |\phi_{jj'}\rangle \langle \phi_{jj'}| \quad (75)$$

and

$$\text{tr}^{\bar{S}} \hat{\rho}_{\text{gmc}} = \frac{1}{d_{\text{gmc}}} \sum_{(j, j') \in \mathcal{J}_{\text{gmc}}} \text{tr}^{\bar{S}} |\phi_{jj'}\rangle \langle \phi_{jj'}| \quad (76a)$$

$$= \frac{1}{d_{\text{gmc}}} \sum_{(j, j') \in \mathcal{J}_{\text{gmc}}} |\phi_j^S\rangle \langle \phi_j^S| \quad (76b)$$

$$= \sum_{j \in \mathcal{J}^S} \frac{\#\{j' \in \mathcal{J}^{\bar{S}} : (j, j') \in \mathcal{J}_{\text{gmc}}\}}{d_{\text{gmc}}} |\phi_j^S\rangle \langle \phi_j^S| \quad (76c)$$

$$= \sum_{j \in \mathcal{J}^S} \frac{\#\{j' \in \mathcal{J}^{\bar{S}} : \forall k : q_{kj'}^{\bar{S}} \in [Q_k - q_{kj}^S - \Delta Q_k, Q_k - q_{kj}^S]\}}{d_{\text{gmc}}} |\phi_j^S\rangle \langle \phi_j^S| \quad (76d)$$

$$= \sum_{j \in \mathcal{J}^S} \frac{\dim \mathcal{H}_j^{\bar{S}}}{d_{\text{gmc}}} |\phi_j^S\rangle \langle \phi_j^S|, \quad (76e)$$

where $\#M$ means the number of elements of the set M and

$$\mathcal{H}_j^{\bar{S}} := \prod_{k=1}^K \mathbb{1}_{[Q_k - q_{kj}^S - \Delta Q_k, Q_k - q_{kj}^S]} (\hat{Q}_k^{\bar{S}}) \mathcal{H}^{\bar{S}}. \quad (77)$$

The Boltzmann entropy of the macro state of $\bar{S}$ defined by the values $q_k^{\bar{S}}$ with tolerance ΔQ_k is defined by [21, 20]

$$S(q_1^{\bar{S}}, \dots, q_K^{\bar{S}}) := k_B \log \dim \left(\prod_{k=1}^K \mathbb{1}_{[q_k^{\bar{S}} - \Delta Q_k, q_k^{\bar{S}}]} (\hat{Q}_k^{\bar{S}}) \mathcal{H}^{\bar{S}} \right), \quad (78)$$

so that

$$\dim \mathcal{H}_j^{\bar{S}} = \exp \left(\frac{1}{k_B} S(Q_1 - q_{1j}^S, \dots, Q_K - q_{Kj}^S) \right). \quad (79)$$

We now approximate the S function in (79) by its Taylor expansion around $(Q_1, \dots, Q_K)$. If the $\hat{Q}_k, \hat{Q}_k^S$ are positive operators, this can be justified as follows: Since S is small, $\bar{S}$

is large compared to S , and positive extensive observables should be dominated by the contribution from $\bar{S}$, so that, for most $(j, j') \in \mathcal{J}_{\text{gmc}}$ and all k ,

$$q_{kj}^S \ll q_{kj'}^{\bar{S}} \approx q_{kj}^S + q_{kj'}^{\bar{S}} \approx Q_k. \quad (80)$$

For $\hat{Q}_k$ that is not positive but merely (as we assumed in Statement 1a) bounded from below, say by $-C_k$, shifting by C_k would justify the Taylor expansion, which then also applies without the shift. We thus obtain, as the first-order Taylor expansion,

$$S(Q_1 - q_{1j}^S, \dots, Q_K - q_{Kj}^S) \approx S(Q_1, \dots, Q_K) - \sum_{k=1}^K \frac{\partial S}{\partial q_k^{\bar{S}}}(Q_1, \dots, Q_K) q_{kj}^S. \quad (81)$$

Inserting into (79) yields

$$\dim \mathcal{H}_j^{\bar{S}} \approx \exp(S(Q_1, \dots, Q_K)/k_B) \exp\left(\sum_{k=1}^K \lambda_k q_{kj}^S\right) \quad (82)$$

with

$$\lambda_k := -\frac{1}{k_B} \frac{\partial S}{\partial q_k^{\bar{S}}}(Q_1, \dots, Q_K). \quad (83)$$

Inserting in (76e) and applying functional calculus of operators,

$$\text{tr}^{\bar{S}} \hat{\rho}_{\text{gmc}} \approx \frac{1}{Z_{\text{gG}}} \exp\left(\sum_{k=1}^K \lambda_k \hat{Q}_k^S\right), \quad (84)$$

which is the definition of $\hat{\rho}_{\text{gG}}^S$.

For the next steps, we need the following mathematical fact, proved in Appendix D.

Proposition 1. *Let $\mathcal{H}^a, \mathcal{H}^b, \mathcal{H}^c$ be finite-dimensional Hilbert spaces. If for some operators*

$$\hat{Q}^a \otimes \hat{I}^b \otimes \hat{I}^c + \hat{I}^a \otimes \hat{Q}^{bc} = \hat{Q}^{ab} \otimes \hat{I}^c + \hat{I}^a \otimes \hat{I}^b \otimes \hat{Q}^c, \quad (85)$$

then there exists a unique operator $\hat{Q}^b$ such that

$$\hat{Q}^{bc} = \hat{Q}^b \otimes \hat{I}^c + \hat{I}^b \otimes \hat{Q}^c \quad (86a)$$

$$\hat{Q}^{ab} = \hat{Q}^a \otimes \hat{I}^b + \hat{I}^a \otimes \hat{Q}^b. \quad (86b)$$

As a consequence, if $S_1 \subseteq S_2 \subseteq \Lambda$, then from (13) for S_1 and S_2 we obtain that

$$\begin{aligned} \hat{Q}_k &\approx \hat{Q}_k^{S_1} \otimes \hat{I}^{S_2 \setminus S_1} \otimes \hat{I}^{\bar{S}_2} \\ &\quad + \hat{I}^{S_1} \otimes \hat{Q}_k^{S_2 \setminus S_1} \otimes \hat{I}^{\bar{S}_2} \\ &\quad + \hat{I}^{S_1} \otimes \hat{I}^{S_2 \setminus S_1} \otimes \hat{Q}_k^{\bar{S}_2}, \end{aligned} \quad (87)$$

and (by repeated application of Proposition 1) similarly for any finite partition $\Lambda = \cup_{\alpha} S_{\alpha}$ ($S_{\alpha} \cap S_{\alpha'} = \emptyset$ for $\alpha \neq \alpha'$):

$$\hat{Q}_k \approx \sum_{\alpha} \hat{Q}_k^{S_{\alpha}} \otimes \hat{I}^{\bar{S}_{\alpha}}. \quad (88)$$

For the derivation of Statement 1a, it remains to verify that λ_k given by (83) agrees (approximately) with λ_k solving (10). Starting from (83), subdividing the available volume Λ into many small regions S_α and using (88), we find that

$$\text{tr}(\hat{\rho}_{\text{gG}} \hat{Q}_k) \approx \sum_{\alpha} \text{tr} \left[\hat{\rho}_{\text{gG}} (\hat{Q}_k^{S_\alpha} \otimes \hat{I}^{\bar{S}_\alpha}) \right] \quad (89a)$$

$$= \sum_{\alpha} \text{tr} \left[\text{tr}^{\bar{S}_\alpha}(\hat{\rho}_{\text{gG}}) \hat{Q}_k^{S_\alpha} \right] \quad (89b)$$

$$\approx \sum_{\alpha} \text{tr} \left[\text{tr}^{\bar{S}_\alpha}(\hat{\rho}_{\text{gmc}}) \hat{Q}_k^{S_\alpha} \right] \quad (89c)$$

$$= \sum_{\alpha} \text{tr} \left[\hat{\rho}_{\text{gmc}} (\hat{Q}_k^{S_\alpha} \otimes \hat{I}^{\bar{S}_\alpha}) \right] \quad (89d)$$

$$= \text{tr}(\hat{\rho}_{\text{gmc}} \hat{Q}_k) \quad (89e)$$

$$\approx Q_k. \quad (89f)$$

Thus, the λ_k given by (83) satisfy (10). This completes the derivation of Statement 1a.

6 Derivation of Statements 2a and 2b: Grand-Canonical Typicality

Statement 2b follows from 1b and 2a together, so we focus on the derivation of 2a. It is based on a theorem of Popescu, Short and Winter [36], often applied to the micro-canonical subspace but proved there for a general subspace³ $\mathcal{H}_R$: *for any $\mathcal{H}^S, \mathcal{H}^B$ of finite dimension, any high-dimensional subspace $\mathcal{H}_R \subseteq \mathcal{H}^S \otimes \mathcal{H}^B$, and most $\Psi \in \mathbb{S}(\mathcal{H}_R)$,*

$$\text{tr}^B |\Psi\rangle\langle\Psi| \approx \text{tr}^B \hat{\rho}_R \quad (90)$$

with $\hat{\rho}_R = (\dim \mathcal{H}_R)^{-1} \hat{P}_R$ the normalized projection to $\mathcal{H}_R$.

(The precise statement is that for every $\eta > 0$,

$$u_{\mathbb{S}(\mathcal{H}_R)} \left\{ \Psi \in \mathbb{S}(\mathcal{H}_R) : \left\| \text{tr}^B |\Psi\rangle\langle\Psi| - \text{tr}^B \hat{\rho}_R \right\|_{\text{tr}} \geq \eta + \frac{d^S}{\sqrt{d_R}} \right\} \leq 4 \exp \left(-\frac{\eta^2 d_R}{18\pi^3} \right) \quad (91)$$

with $d^S = \dim \mathcal{H}^S$, $d_R = \dim \mathcal{H}_R$, and $\|\hat{M}\|_{\text{tr}} = \text{tr} |\hat{M}| = \text{tr} \sqrt{\hat{M}^* \hat{M}}$ the trace norm of the operator $\hat{M}$.)

Applying this to $\mathcal{H}_R := \mathcal{H}_{\text{gmc}}$ with $B = \bar{S}$ and using that $\dim \mathcal{H}_{\text{gmc}}$ is large, we obtain that for most $\Psi \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$,

$$\text{tr}^{\bar{S}} |\Psi\rangle\langle\Psi| \approx \text{tr}^{\bar{S}} \hat{\rho}_{\text{gmc}}. \quad (92)$$

By Statement 1a, $\text{tr}^{\bar{S}} \hat{\rho}_{\text{gmc}} \approx \hat{\rho}_{\text{gG}}^S$, which yields the desired result.

³Indeed, as they put it in [36], p.3: “Furthermore our principle will apply to arbitrary restrictions R that have nothing to do with energy, which may lead to many interesting insights.” As parts of our paper show, this is the case.

7 Derivation of Statements 3, 4a, 4b: Conditional Wave Function and GAP

Before deriving Statements 3–5, we review the properties of the GAP measure (for a pedagogical introduction see [52]).

7.1 GAP Measure

GAP measures can arise in several ways [19, 17]; the one most relevant to us is as the asymptotic distribution of the conditional wave function ψ^S in the setting of canonical typicality (leading to (4b)) and, of course, according to Statements 3–4b. That is, GAP measures are relevant as the distribution of wave functions for Gibbs ensembles.

For any Hilbert space $\mathcal{H}$ and probability measure μ on $\mathbb{S}(\mathcal{H})$, the density matrix of μ is

$$\hat{\rho}_\mu = \int_{\mathbb{S}(\mathcal{H})} \mu(d\psi) |\psi\rangle\langle\psi|. \quad (93)$$

Note that the map $\mu \mapsto \hat{\rho}_\mu$ is many-to-one; there are several measures leading to the same density matrix. For any $\hat{\rho}$, $\text{GAP}_{\hat{\rho}}$ is a particular measure with density matrix $\hat{\rho}$, i.e.,

$$\hat{\rho}_{\text{GAP}_{\hat{\rho}}} = \hat{\rho}. \quad (94)$$

In fact, $\text{GAP}_{\hat{\rho}}$ is the most spread-out measure with given $\hat{\rho}$ [25]. The name stems from a procedure for constructing it: G stands for Gaussian, A for adjusted and P for projected. Here is the procedure:

We write $X \sim p$ to express that the random variable X has probability distribution p . Let $\hat{\rho} = \sum_m p_m |m\rangle\langle m|$ be a density matrix on a finite-dimensional Hilbert space $\mathcal{H}$ with eigenvalues p_m and corresponding eigen-ONB $\{|m\rangle\}$. Moreover, let (Z_m) be a sequence of independent complex-valued Gaussian random variables⁴ with mean 0 and variances

$$\mathbb{E}|Z_m|^2 = p_m. \quad (95)$$

Then $G_{\hat{\rho}}$ is the distribution of the random vector

$$\Psi^G := \sum_m Z_m |m\rangle. \quad (96)$$

Note that while $G_{\hat{\rho}}$ has density matrix $\hat{\rho}$, it is not a distribution on the sphere $\mathbb{S}(\mathcal{H})$. However, as the eigenvalues p_m sum up to 1, we immediately see that $\mathbb{E}\|\Psi^G\|^2 = 1$.

If we now projected the Gaussian measure $G_{\hat{\rho}}$ to the sphere $\mathbb{S}(\mathcal{H})$, the resulting distribution would in general not have density matrix $\hat{\rho}$. In order to obtain a measure with the desired density matrix after projecting to the sphere, we have to adjust the density of $G_{\hat{\rho}}$. More precisely, we define the Gaussian adjusted measure $\text{GA}_{\hat{\rho}}$ on $\mathcal{H}$ by

$$\text{GA}_{\hat{\rho}}(d\psi) = \|\psi\|^2 G_{\hat{\rho}}(d\psi). \quad (97)$$

⁴Recall that Z is a complex-valued Gaussian random variable with mean μ and variance σ^2 if and only if $\text{Re}Z$ and $\text{Im}Z$ are independent and $\text{Re}Z \sim \mathcal{N}(\text{Re}\mu, \sigma^2/2)$, $\text{Im}Z \sim \mathcal{N}(\text{Im}\mu, \sigma^2/2)$.

We remark that because of $\mathbb{E}\|\Psi^G\|^2 = 1$, $\text{GA}_{\hat{\rho}}$ defines indeed a probability distribution on $\mathcal{H}$.

In the last step of the construction we project $\text{GA}_{\hat{\rho}}$ to $\mathbb{S}(\mathcal{H})$. Let $\Psi^{\text{GA}} \sim \text{GA}_{\hat{\rho}}$. Then $\text{GAP}_{\hat{\rho}}$ is the distribution of the random vector

$$\Psi^{\text{GAP}} := \frac{\Psi^{\text{GA}}}{\|\Psi^{\text{GA}}\|}. \quad (98)$$

Note that Ψ^{GAP} is well-defined as $\Psi^{\text{GA}} \neq 0$ almost surely. One can easily see that indeed $\hat{\rho}_{\text{GAP}_{\hat{\rho}}} = \hat{\rho}$ and thus this concludes the construction of GAP measures in the finite-dimensional setting. If $\mathcal{H}$ is infinite-dimensional, a similar construction is possible, see [53] for the details. For other constructions of $\text{GAP}_{\hat{\rho}}$, see [17].

Another property we use is the continuous dependence of $\text{GAP}_{\hat{\rho}}$ on $\hat{\rho}$, which means that for two density matrices $\hat{\rho}, \hat{\Omega}$,

$$\text{if } \hat{\rho} \approx \hat{\Omega}, \text{ then } \text{GAP}_{\hat{\rho}} \approx \text{GAP}_{\hat{\Omega}}. \quad (99)$$

A precise version is provided by Lemma 5 in [17], which says that for every $0 < \varepsilon < 1$, every finite-dimensional $\mathcal{H}$, and every continuous function $f : \mathbb{S}(\mathcal{H}) \rightarrow \mathbb{R}$, there is $r = r(\varepsilon, \dim \mathcal{H}, f) > 0$ such that for all $\hat{\rho}, \hat{\Omega} \in \mathcal{D}(\mathcal{H})$

$$\text{if } \|\hat{\rho} - \hat{\Omega}\|_{\text{tr}} < r, \text{ then } |\text{GAP}_{\hat{\rho}}(f) - \text{GAP}_{\hat{\Omega}}(f)| < \varepsilon. \quad (100)$$

Here, we used a standard way of expressing the closeness of two measures μ, ν on a set Ω by saying that for any function $f : \Omega \rightarrow \mathbb{R}$ (serving as a “test function”), the μ -average of f

$$\mu(f) := \int_{\Omega} \mu(d\omega) f(\omega) \quad (101)$$

is close to $\nu(f)$. Different classes of test functions (e.g., bounded, continuous) define different types of closeness.

Further investigation and discussion of GAP measures can be found in [19, Sec. 3], [54, 38, 17, 50, 56].

7.2 Derivation of Statement 3

The key ingredient is Theorem 2 from [17], which says that *for any finite-dimensional $\mathcal{H}^S, \mathcal{H}^B$ with large $\dim \mathcal{H}^B$ and any $\Psi \in \mathbb{S}(\mathcal{H}^S \otimes \mathcal{H}^B)$, most ONBs b of $\mathcal{H}^B$ are such that*

$$\mathcal{L}_{\psi^S} \approx \text{GAP}_{\text{tr}^B |\Psi\rangle\langle\Psi|}. \quad (102)$$

(More precisely, it says that for every $\varepsilon > 0$, $d^B := \dim \mathcal{H}^B \geq \max\{4, \dim \mathcal{H}^S\}$, $\Psi \in \mathbb{S}(\mathcal{H}^S \otimes \mathcal{H}^B)$, and bounded measurable test function $f : \mathbb{S}(\mathcal{H}^S) \rightarrow \mathbb{R}$,

$$u_{\text{ONB}} \left\{ b : |\mathcal{L}_{\psi^S}(f) - \text{GAP}_{\text{tr}^B |\Psi\rangle\langle\Psi|}(f)| < \varepsilon \|f\|_{\infty} \right\} \geq 1 - \frac{4}{\varepsilon^2 d^B} \quad (103)$$

with u_{ONB} the uniform distribution over the set of ONBs of $\mathcal{H}^B$ and $\|\cdot\|_{\infty}$ the supremum norm.)

We apply this to $B = \bar{S}$. By Statement 2a, for most $\Psi \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$, $\text{tr}^B |\Psi\rangle\langle\Psi| \approx \hat{\rho}_{\text{gG}}^S$. By (99),⁵ $\text{GAP}_{\text{tr}^B |\Psi\rangle\langle\Psi|} \approx \text{GAP}_{\hat{\rho}_{\text{gG}}^S}$. Thus, $\mathcal{L}_{\psi^S} \approx \text{GAP}_{\hat{\rho}_{\text{gG}}^S}$ as claimed (and likewise in the setting of Statement 2b).

Remark 7. Another reasoning leads to the related result that $\mathcal{L}_{\psi^S}$, when *averaged* over $\Psi \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$, is close to $\text{GAP}_{\hat{\rho}_{\text{gG}}^S}$. It is based on the property [19, Sec. 3, Property 3] that “GAP is hereditary,” i.e., that if $\Psi \in \mathbb{S}(\mathcal{H}^S \otimes \mathcal{H}^B)$ has distribution $\text{GAP}_{\hat{\rho}^S \otimes \hat{\rho}^B}$, then for any fixed ONB b of $\mathcal{H}^B$, $\mathbb{E}_{\Psi} \mathcal{L}_{\psi^S} = \text{GAP}_{\hat{\rho}^S}$. The difference to (102) is twofold: First, the equality is exact, not approximate; and second, it concerns the *average* over Ψ , while (102) is the case for *most* Ψ . For our application, the exactness does not help as it gets lost in other steps. The application here looks as follows: Suppose that $\hat{\rho}_{\text{gmc}} \approx \hat{\rho}_{\text{gG}}$. Then the typicality measure for Ψ is $u_{\mathbb{S}(\mathcal{H}_{\text{gmc}})} = \text{GAP}_{\hat{\rho}_{\text{gmc}}} \approx \text{GAP}_{\hat{\rho}_{\text{gG}}} \approx \text{GAP}_{\hat{\rho}_{\text{gG}}^S \otimes \hat{\rho}_{\text{gG}}^{\bar{S}}}$ by (40) and (99). By hereditary, for any ONB b of $\mathcal{H}^{\bar{S}}$, $\mathbb{E}_{\Psi} \mathcal{L}_{\psi^S} \approx \text{GAP}_{\hat{\rho}_{\text{gG}}^S}$. $\diamond$

7.3 Derivation of Statement 4a

An ONB diagonalizing certain commuting observables $\hat{A}_1, \dots, \hat{A}_n$ (such as $\hat{Q}_1^{\bar{S}}, \dots, \hat{Q}_{K-1}^{\bar{S}}$ or later $\hat{N}_1^{\bar{S}}, \dots, \hat{N}_r^{\bar{S}}$) consists of an ONB for each of their joint eigenspaces (which in the relevant cases will have high dimension). Thus, a purely random ONB diagonalizing $\hat{A}_1, \dots, \hat{A}_n$ consists of a purely random ONB in each of the joint eigenspaces. Since the construction of ψ^S involves picking a random basis vector b_J , and since each basis vector lies in one of the joint eigenspaces, we ask what is the probability that the chosen basis vector lies in a particular joint eigenspace (say, the one with eigenvalues $a_1, \dots, a_n$, denoted $\mathcal{H}_{a_1 \dots a_n}$). Since

$$\mathbb{P}(J = j) = \|\langle b_j | \Psi \rangle_B\|_S^2 \quad (104a)$$

$$= \langle \Psi | (\hat{I}^S \otimes |b_j\rangle\langle b_j|) | \Psi \rangle_{S \cup B}, \quad (104b)$$

we find that, given a basis b ,

$$\mathbb{P}(b_J \in \mathcal{H}_{a_1 \dots a_n} | b) = \sum_{j: b_j \in \mathcal{H}_{a_1 \dots a_n}} \mathbb{P}(J = j) \quad (105a)$$

$$= \left\langle \Psi \left| \left(\hat{I}^S \otimes \sum_{j: b_j \in \mathcal{H}_{a_1 \dots a_n}} |b_j\rangle\langle b_j| \right) \right| \Psi \right\rangle \quad (105b)$$

$$= \langle \Psi | (\hat{I}^S \otimes \hat{P}_{a_1 \dots a_n}) | \Psi \rangle =: \tilde{p}(a_1, \dots, a_n), \quad (105c)$$

which is independent of the choice of basis b , as it depends only on the projection $\hat{P}_{a_1 \dots a_n}$ to the joint eigenspace. As a consequence, the random variable ψ^S can be constructed from a given Ψ as follows: instead of first choosing a basis b diagonalizing $\hat{A}_1, \dots, \hat{A}_n$ in all of $\mathcal{H}^B$ and then a random J with Born distribution, we can just as well choose first a joint eigenspace $\mathcal{H}_{a_1 \dots a_n}$ with Born distribution (105c), then a random ONB b' in this

⁵Theorems 3 and 4 in [17] provide precise versions of this reasoning.

subspace, and then one basis vector $b'_{j'}$ with conditional Born distribution, given that the eigenspace was $\mathcal{H}_{a_1 \dots a_n}$. Finally, we can form

$$\psi^S = \mathcal{N} \langle b'_{j'} | \Psi \rangle. \quad (106)$$

This conditional Born distribution is exactly the Born distribution associated with

$$\Psi' = \frac{(\hat{I}^S \otimes \hat{P}_{a_1 \dots a_n}) \Psi}{\|(\hat{I}^S \otimes \hat{P}_{a_1 \dots a_n}) \Psi\|}, \quad (107)$$

which can be thought of as the collapsed wave function after a simultaneous quantum measurement of $\hat{A}_1, \dots, \hat{A}_n$ on Ψ with outcomes $a_1, \dots, a_n$. Since $b'_{j'} \in \mathcal{H}_{a_1 \dots a_n}$, ψ^S can just as well be obtained from Ψ' instead of Ψ ,

$$\psi^S = \mathcal{N}' \langle b'_{j'} | \Psi' \rangle \quad (108)$$

with different normalizing constant $\mathcal{N}'$. That is, after choosing $a_1, \dots, a_n$ with Born distribution, we can simply continue with Ψ' , so that $\mathcal{H}^B$ gets replaced by $\mathcal{H}_{a_1 \dots a_n}$. In particular, Theorem 2 of [17] (as described around (102) above) can be applied as long as $\dim \mathcal{H}_{a_1 \dots a_n} \gg 1$, and yields that for most ONBs b' of $\mathcal{H}_{a_1 \dots a_n}$, the distribution of ψ^S is approximately $\text{GAP}_{\text{tr}^B |\Psi'\rangle\langle\Psi'|}$. Thus, including all possible values of $a_1, \dots, a_n$,

$$\mathcal{L}_{\psi^S} \approx \bigoplus_{a_1 \dots a_n} \tilde{p}(a_1, \dots, a_n) \text{GAP}_{\text{tr}^B |\Psi'\rangle\langle\Psi'|}. \quad (109)$$

We now apply this to the setting of Statement 4a. Since

$$\Psi \in \mathcal{H}_{\text{gmc}} \subset \widetilde{\mathcal{H}} := \prod_{k=1}^{K-1} \mathbb{1}_{\{Q_k\}}(\hat{Q}_k) \mathcal{H} \quad (110a)$$

$$= \bigoplus_{q_1^S \dots q_{K-1}^S} \left(\prod_{k=1}^{K-1} \mathbb{1}_{\{q_k^S\}}(\hat{Q}_k^S) \mathcal{H}^S \right) \otimes \left(\prod_{k=1}^{K-1} \mathbb{1}_{\{Q_k - q_k^S\}}(\hat{Q}_k^{\bar{S}}) \mathcal{H}^{\bar{S}} \right), \quad (110b)$$

we have that

$$\left(\hat{P}(\hat{Q}_1^S = q_1^S, \dots) \otimes \hat{I}^{\bar{S}} \right) \Big|_{\widetilde{\mathcal{H}}} = \left(\hat{I}^S \otimes \hat{P}(\hat{Q}_1^{\bar{S}} = Q_1 - q_1^S, \dots) \right) \Big|_{\widetilde{\mathcal{H}}}. \quad (111)$$

Thus,

$$\tilde{p}(Q_1 - q_1^S, \dots) = p(q_1^S, \dots) \quad (112)$$

as defined in (57), and (taking $\hat{P}(\dots)$ to mean operators on $\mathcal{H}$ or $\mathcal{H}^S$ or $\mathcal{H}^{\bar{S}}$ depending on the context)

$$\text{tr}^{\bar{S}} |\Psi'\rangle\langle\Psi'| = (\mathcal{N}')^2 \text{tr}^{\bar{S}} \left(\hat{P}(\hat{Q}_1^{\bar{S}} = Q_1 - q_1^S, \dots) |\Psi\rangle\langle\Psi| \hat{P}(\hat{Q}_1^{\bar{S}} = Q_1 - q_1^S, \dots) \right) \quad (113a)$$

$$= (\mathcal{N}')^2 \text{tr}^{\bar{S}} \left(\hat{P}(\hat{Q}_1^S = q_1^S, \dots) |\Psi\rangle\langle\Psi| \hat{P}(\hat{Q}_1^S = q_1^S, \dots) \right) \quad (113b)$$

$$= (\mathcal{N}')^2 \hat{P}(\hat{Q}_1^S = q_1^S, \dots) \text{tr}^{\bar{S}} (|\Psi\rangle\langle\Psi|) \hat{P}(\hat{Q}_1^S = q_1^S, \dots) \quad (113c)$$

$$\approx (\mathcal{N}')^2 \hat{P}(\hat{Q}_1^S = q_1^S, \dots) \hat{\rho}_{\text{gG}}^S \hat{P}(\hat{Q}_1^S = q_1^S, \dots) = (58) \quad (113d)$$

for most $\Psi \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$ by Statement 2a. By (99), we obtain Statement 4a.

7.4 Derivation of Statement 4b

We apply (109) to $n = r$ and $\hat{A}_i = \hat{N}_i^{\bar{S}}$. By Theorem 1 in [49] for $t = 0$, for most $\Psi \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$, $\tilde{p}(n_1^{\bar{S}}, \dots, n_r^{\bar{S}}) \approx \text{tr}(\hat{\rho}_{\text{gmc}} \hat{P}_n) = p_n(n_1^{\bar{S}}, \dots, n_r^{\bar{S}})$. Given $n_1^{\bar{S}}, \dots, n_r^{\bar{S}}$, Ψ' is GAP-distributed with density matrix $\hat{P}_n \hat{\rho}_{\text{gmc}} \hat{P}_n / p_n(n_1^{\bar{S}}, \dots, n_r^{\bar{S}})$. (This can be shown.) By the results of [50], $\text{tr}^{\bar{S}} |\Psi'\rangle \langle \Psi'| \approx \hat{\rho}(n_1^{\bar{S}}, \dots, n_r^{\bar{S}})$ with probability close to 1. Thus, (109) takes the form (59). This completes the derivation of Statement 4b.

Remark 5 can now be obtained as follows: When acting on $\mathcal{H}_{\text{gmc}}$, $\hat{I}^S \otimes \hat{P}_n$ can be replaced by $\hat{P} \otimes \hat{P}_n$ with $\hat{P}$ as in (57) and $q_k^S := Q_k - F_k(n_1^{\bar{S}}, \dots, n_r^{\bar{S}})$. Given that we can otherwise replace $\hat{\rho}_{\text{gmc}}$ by $\hat{\rho}_{\text{gG}} \approx \hat{\rho}_{\text{gc}}$, and using (40), we find that

$$p_n(n_1^{\bar{S}}, \dots, n_r^{\bar{S}}) = \text{tr}[\hat{\rho}_{\text{gmc}}(\hat{I}^S \otimes \hat{P}_n)] \quad (114a)$$

$$= \text{tr}[\hat{\rho}_{\text{gmc}}(\hat{P} \otimes \hat{P}_n)] \quad (114b)$$

$$\approx \text{tr}[\hat{\rho}_{\text{gG}}(\hat{P} \otimes \hat{P}_n)] \quad (114c)$$

$$= \text{tr}(\hat{\rho}_{\text{gG}}^S \hat{P}) \text{tr}(\hat{\rho}_{\text{gG}}^{\bar{S}} \hat{P}_n) \quad (114d)$$

and in the same way $\hat{\rho}(n_1^{\bar{S}}, \dots, n_r^{\bar{S}}) \approx \hat{\rho}^S(q_1^S, \dots, q_{K-1}^S)$ as in (58). Thus, all summands in (59) with equal values of $q_1^S, \dots, q_{K-1}^S$ are multiples of the same distribution $\text{GAP}_{\hat{\rho}^S(q_1^S, \dots, q_{K-1}^S)}$, and thus can be combined into a single summand with weight

$$\sum_{\substack{n_1^{\bar{S}} \dots n_r^{\bar{S}}: \\ Q_k - F_k(n_1^{\bar{S}}, \dots, n_r^{\bar{S}}) = q_k^S}} p_n(n_1^{\bar{S}}, \dots, n_r^{\bar{S}}) \approx \text{tr}(\hat{\rho}_{\text{gG}}^S \hat{P}) = p(q_1^S, \dots, q_{K-1}^S), \quad (115)$$

which leads to the equations of Remark 5.

Example 2. As a simple example we consider the case of one particle species ($r = 1$). In this situation there is no notion of chemical equilibrium but only the one of spatial equilibrium.

Let $\mathcal{H} = \mathcal{H}^S \otimes \mathcal{H}^{\bar{S}}$ and let $\hat{Q}_1 = \hat{N}$ be the particle number operator of the total system. Obviously, $\hat{N}$ is (exactly) extensive and thus we can decompose it as

$$\hat{N} = \hat{N}^S \otimes \hat{I}^{\bar{S}} + \hat{I}^S \otimes \hat{N}^{\bar{S}}, \quad (116)$$

where $\hat{N}^S$ and $\hat{N}^{\bar{S}}$ are the particle number operators of S and $\bar{S}$, with eigenvalues n^S and $n^{\bar{S}}$, acting on $\mathcal{H}^S$ and $\mathcal{H}^{\bar{S}}$ respectively.

Let $\Delta N = 0$ and let $N \in \mathbb{N}$ be an eigenvalue of $\hat{N}$, so $\mathcal{H}_{\text{gmc}}$ is characterized by the (exact) total particle number and a micro-canonical energy interval. By Statement 4b, for most $\Psi \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$ and most ONBs b of $\mathcal{H}^{\bar{S}}$ that diagonalize $\hat{N}^{\bar{S}}$,

$$\mathcal{L}_{\psi^S} \approx \bigoplus_{n^{\bar{S}}=0}^N p_n(n^{\bar{S}}) \text{GAP}_{\hat{\rho}(n^{\bar{S}})}, \quad (117)$$

where

$$p_n(n^{\bar{S}}) = \text{tr}(\hat{\rho}_{\text{gmc}} \hat{P}_n), \quad \hat{\rho}(n^{\bar{S}}) = \frac{1}{p_n(n^{\bar{S}})} \text{tr}^{\bar{S}} \left[\hat{P}_n \hat{\rho}_{\text{gmc}} \hat{P}_n \right], \quad (118)$$

with $\hat{P}_n = \hat{P}(\hat{N}^{\bar{S}} = n^{\bar{S}})$. These quantities can be evaluated more explicitly: with the help of (111) and Statement 1b we find that

$$p_n(n^{\bar{S}}) = \text{tr} \left(\left(\hat{P}(\hat{N}^S = N - n^{\bar{S}}) \otimes \hat{I}^{\bar{S}} \right) \hat{\rho}_{\text{gmc}} \right) \quad (119a)$$

$$= \text{tr}^S \left(\hat{P}(\hat{N}^S = N - n^{\bar{S}}) \text{tr}^{\bar{S}}(\hat{\rho}_{\text{gmc}}) \right) \quad (119b)$$

$$\approx \frac{1}{Z_{\text{gc}}} \text{tr}^S \left(\hat{P}(\hat{N}^S = N - n^{\bar{S}}) \text{tr}^{\bar{S}} \left(e^{-\beta(\hat{H}_0 - \mu \hat{N})} \right) \right) \quad (119c)$$

$$= \frac{1}{Z_{\text{gc}}^S} e^{\beta\mu(N - n^{\bar{S}})} \text{tr}^S \left(\hat{P}(\hat{N}^S = N - n^{\bar{S}}) e^{-\beta\hat{H}_0^S} \right), \quad (119d)$$

where $\hat{H}_0^S$ is the part of $\hat{H}_0$ acting only on S and $\mu = \mu_{01}$. Likewise,

$$\hat{\rho}(n^{\bar{S}}) = \frac{1}{p_n(n^{\bar{S}})} \text{tr}^{\bar{S}} \left(\hat{P}(\hat{N}^{\bar{S}} = n^{\bar{S}}) \hat{\rho}_{\text{gmc}} \right) \quad (120a)$$

$$= \frac{1}{p_n(n^{\bar{S}})} \hat{P}(\hat{N}^S = N - n^{\bar{S}}) \left(\text{tr}^{\bar{S}} \hat{\rho}_{\text{gmc}} \right) \hat{P}(\hat{N}^S = N - n^{\bar{S}}) \quad (120b)$$

$$\approx \frac{1}{Z_{\text{gc}}^S} \frac{1}{p_n(n^{\bar{S}})} \hat{P}(\hat{N}^S = N - n^{\bar{S}}) e^{-\beta(\hat{H}_0^S - \mu \hat{N}^S)} \hat{P}(\hat{N}^S = N - n^{\bar{S}}) \quad (120c)$$

$$= \frac{1}{Z_{\text{gc}}^S p_n(n^{\bar{S}})} e^{\beta\mu(N - n^{\bar{S}})} \hat{P}(\hat{N}^S = N - n^{\bar{S}}) e^{-\beta\hat{H}_0^S} \hat{P}(\hat{N}^S = N - n^{\bar{S}}). \quad (120d)$$

Therefore, $\hat{\rho}(n^{\bar{S}})$ can be interpreted as a canonical density matrix of the system S with $N - n^{\bar{S}}$ particles and thus (117) is a mixture of GAP measures with canonical density matrices corresponding to different particle numbers in S .

As a by-product, we observe that (63) reduces in this example to (119d) with $q_1^S = n^S = N - n^{\bar{S}}$ because $\hat{Q}_1 = \hat{N}$, and (64) reduces to (120d). Thus, the calculation above amounts to an independent confirmation of Remark 5 in this case that does not assume the validity of the general Gibbs principle. $\diamond$

8 Derivation of Statement 5: Approach to Equilibrium

For deriving Statement 5, we make use of the following three mathematical propositions.

The first one provides a large part of the first statement in Statement 5: it states that a version of the eigenstate thermalization hypothesis (ETH) suitable for microscopic thermal equilibrium (MITE) implies that the reduced density matrix $\hat{\rho}_{\Psi_t}^S$ approaches $\text{tr}^{\bar{S}} \hat{\rho}_{\text{gmc}}$ for every initial state $\Psi_0 \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$. The MITE-ETH was formulated in Statement 5 as (65a) and (65b) and is formulated in Proposition 2 in a more precise version as (123) and (124).

For the mathematical formulation, we recall the precise meaning of “most” [57, 16]: One says that a statement $s(x)$ is true *for* $(1 - \varepsilon)$ -most $x \in X$ relative to the normalized measure μ on X if and only if

$$\mu\{x \in X : s(x)\} \geq 1 - \varepsilon. \quad (121)$$

One says that a statement $s(t)$ is true *for* $(1 - \varepsilon)$ -most $t \in [0, \infty)$ if and only if

$$\liminf_{T \rightarrow \infty} \frac{1}{T} \left| \{t \in [0, \infty) : s(t)\} \right| \geq 1 - \varepsilon, \quad (122)$$

where $|M|$ denotes the length (Lebesgue measure) of the set $M \subseteq \mathbb{R}$.

Proposition 2. *Let $\varepsilon, \delta > 0$, $\mathcal{H} = \mathcal{H}^S \otimes \mathcal{H}^B$, let $\mathcal{H}_R \subset \mathcal{H}$ be a subspace, $\hat{P}_R$ the projection to $\mathcal{H}_R$, and $\hat{H}$ a Hamiltonian on $\mathcal{H}$ such that $[\hat{H}, \hat{P}_R] = 0$. Moreover, suppose (MITE-ETH) that for any eigenvectors $\phi_1, \phi_2 \in \mathbb{S}(\mathcal{H}_R)$ of $\hat{H}$ with eigenvalues $e_1 \neq e_2$,*

$$\left\| \text{tr}^B |\phi_1\rangle\langle\phi_1| - \text{tr}^B \hat{\rho}_R \right\|_2 < \varepsilon, \quad (123)$$

$$\left\| \text{tr}^B |\phi_1\rangle\langle\phi_2| \right\|_2 < \varepsilon, \quad (124)$$

where $\|\cdot\|_2$ denotes the Hilbert-Schmidt norm. Then every $\psi_0 \in \mathbb{S}(\mathcal{H}_R)$ is such that for $(1 - \delta)$ -most $t \in [0, \infty)$,

$$\left\| \text{tr}^B |\psi_t\rangle\langle\psi_t| - \text{tr}^B \hat{\rho}_R \right\|_2 < 2\varepsilon \sqrt{\frac{D_G}{\delta}}, \quad (125)$$

where D_G is the maximal degeneracy of eigenvalue gaps,

$$D_G := \max_{E \in \mathbb{R}} \#\{(e, e') \in \mathcal{E} \times \mathcal{E} : e \neq e' \text{ and } e - e' = E\}, \quad (126)$$

and $\mathcal{E}$ the set of eigenvalues of $\hat{H}$.

Proposition 2 expresses that for every initial state $\psi_0 \in \mathbb{S}(\mathcal{H}_R)$, for most times $t \geq 0$, $\hat{\rho}_{\psi_t}^S \approx \text{tr}^B \hat{\rho}_R$. The proof can be found in Appendix E. It is an adaption and generalization of the one given in [48, 39, 14] for the case that $\hat{\rho}_R = \hat{\rho}_{\text{mc}}$ and the Hamiltonian has non-degenerate eigenvalues and eigenvalue gaps.

Another proposition concerns the commutation of quantifiers. It is helpful to introduce the symbol $\forall$ to denote “for most.” If $A(x, y)$ is any statement about objects x and y , then “ $\forall x \forall y : A(x, y)$ ” is equivalent to “ $\forall y \forall x : A(x, y)$.” Likewise, “ $\forall x \forall y : A(x, y)$ ” is equivalent to “ $\forall y \forall x : A(x, y)$ ” [16, Footnote 7] if both $\forall x$ and $\forall y$ refer to probability spaces (i.e., normalized measures); the situation is more subtle when talking about most times $t \in [0, \infty)$ because the uniform measure on $[0, \infty)$ is not normalizable. In fact, “ $\forall x \forall t : A(x, t)$ ” implies that “ $\forall t \forall x : A(x, t)$ ” but in general not vice versa [56, Footnote 5]. The following proposition provides a sufficient condition for commuting $\forall t$ from the left to the right of $\forall x$.

Proposition 3. Suppose $(X, \mathcal{F}, \mathbb{P})$ is a probability space, $C > 0$, $F : X \times [0, \infty) \rightarrow [0, C]$ is a measurable function, $0 < \varepsilon < 1$, $0 < \delta_x < 1$, and $0 < \delta_t < 1$. Suppose further that for every $x \in X$, the time average

$$\overline{F(x, t)} := \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt F(x, t) \text{ exists.} \quad (127)$$

If $(1 - \delta_t)$ -most $t \in [0, \infty)$ are such that for $(1 - \delta_x)$ -most $x \in X$, $F(x, t) \leq \varepsilon$, then $(1 - \delta'_x)$ -most $x \in X$ are such that for $(1 - \delta'_t)$ -most $t \in [0, \infty)$, $F(x, t) \leq \varepsilon'$ with any positive $\varepsilon', \delta'_t, \delta'_x$ such that

$$\varepsilon' \delta'_t \delta'_x \leq \varepsilon + C(\delta_x + \delta_t) \quad (128)$$

(e.g., $\varepsilon' = \delta'_t = \delta'_x = (\varepsilon + C(\delta_x + \delta_t))^{1/3}$).

The proof can be found in Appendix F.

Proposition 4. Let $\mathcal{H}$ be a finite-dimensional Hilbert space, $\Psi_0 \in \mathbb{S}(\mathcal{H})$, $\Psi_t = \exp(-i\hat{H}t)\Psi_0$ with self-adjoint $\hat{H}$, and let $g : \mathbb{S}(\mathcal{H}) \rightarrow \mathbb{R}$ be any bounded measurable function. Then the time average $\overline{g(\Psi_t)}$ exists.

The proof can be found in Appendix G.

Derivation of Statement 5. We assume that $\hat{H}$ satisfies the ETH (123)–(124), and that D_G is not too large. Then Proposition 2 for $\mathcal{H}_R = \mathcal{H}_{\text{gmc}}$ yields that for every $\Psi_0 \in \mathbb{S}(\mathcal{H}_{\text{gmc}})$, for most times $t \in [0, \infty)$, $\hat{\rho}_{\Psi_t}^S \approx \text{tr}^{\bar{S}} \hat{\rho}_{\text{gmc}}$. Statement 1a tells us that $\text{tr}^{\bar{S}} \hat{\rho}_{\text{gmc}} \approx \hat{\rho}_{\text{gG}}^S$. We thus obtain the first statement (66) of Statement 5.

We now turn to the conditional wave function. Theorem 2 in [17] shows that for every t , most orthonormal bases b of $\mathcal{H}^{\bar{S}}$ are such that $\mathcal{L}_{\psi^S(t)} \approx \text{GAP}_{\hat{\rho}_{\Psi_t}^S}$. By the continuous dependence (99) of $\text{GAP}_{\hat{\rho}}$ on $\hat{\rho}$, $\text{GAP}_{\hat{\rho}_{\Psi_t}^S} \approx \text{GAP}_{\hat{\rho}_{\text{gG}}^S}$ for most t and regardless of the basis b . Thus,

$$\forall \Psi_0 \ \forall t \geq 0 \ \forall b : \mathcal{L}_{\psi^S(t)} \approx \text{GAP}_{\hat{\rho}_{\text{gG}}^S}. \quad (129)$$

We want to move the “ $\forall b$ ” to the left of “ $\forall t$ ” because we want to apply the same basis b at all times t . As discussed before Proposition 3, even commuting $\forall t$ and $\forall b$ requires further assumptions, to which we turn now. We express that $\mathcal{L}_{\psi^S(t)}$ is close to $\text{GAP}_{\hat{\rho}_{\text{gG}}^S}$ by means of integrating them against arbitrary “test” functions $f : \mathbb{S}(\mathcal{H}^S) \rightarrow \mathbb{R}$ as in (101). Proposition 3 for $X = \text{ONB}(\mathcal{H}^{\bar{S}})$, $x = b$, and $F(b, t) = |\mathcal{L}_{\psi^S(t)}(f) - \text{GAP}_{\hat{\rho}_{\text{gG}}^S}(f)|$ (which satisfies $0 \leq F(b, t) \leq C = 2\|f\|_\infty$) allows us to interchange $\forall t$ and $\forall b$, as its hypothesis (127) is satisfied by virtue of Proposition 4 with $g(\Psi) = |\mathcal{L}_{\psi^S}(f) - \text{GAP}_{\hat{\rho}_{\text{gG}}^S}(f)|$ (note that ψ^S depends on Ψ) for arbitrary but fixed b and f ; after all, $F(b, t) = g(\Psi_t)$. Thus,

$$\forall \Psi_0 \ \forall b \ \forall t \geq 0 : \mathcal{L}_{\psi^S(t)} \approx \text{GAP}_{\hat{\rho}_{\text{gG}}^S}, \quad (130)$$

which is what we claimed in the case of typical ONBs b ; the case of ONBs diagonalizing $\hat{Q}_1, \dots, \hat{Q}_{K-1}$ is analogous, while $\forall b$ now means “for most ONBs b diagonalizing

$\hat{Q}_1, \dots, \hat{Q}_{K-1}$ ” instead of “for most ONBs b .” This completes the derivation of Statement 5.

An alternative strategy of the derivation starts from the fact, mentioned above, that $\forall \Psi_0 \forall t \geq 0 \forall b : \mathcal{L}_{\psi^S(t)} \approx \text{GAP}_{\hat{\rho}_{\Psi_t}^S}$. Now we try first, before replacing $\hat{\rho}_{\Psi_t}^S$ by $\hat{\rho}_{\text{gG}}^S$, to move “ $\forall b$ ” to the left of the t -quantifier. It must still be expected that “ $\forall t$ ” has to be replaced by the weaker “ $\forall t$ ” because it may well happen that every b has some bad, exceptional t ’s [16]. We apply Proposition 4 to $g(\Psi) = |\mathcal{L}_{\psi^S}(f) - \text{GAP}_{\hat{\rho}_{\Psi}^S}(f)|$, then Proposition 3 to $X = \text{ONB}(\mathcal{H}^{\bar{S}})$, $x = b$, and $F(b, t) = |\mathcal{L}_{\psi^S(t)}(f) - \text{GAP}_{\hat{\rho}_{\Psi_t}^S}(f)| = g(\Psi_t)$, so we can interchange $\forall t$ and $\forall b$. Now if each of two statements $s_1(t)$ and $s_2(t)$ is true for $(1 - \varepsilon)$ -most t , then “ $s_1(t)$ and $s_2(t)$ ” is true for at least $(1 - 2\varepsilon)$ -most t . Since $\forall t : \hat{\rho}_{\Psi_t}^S \approx \hat{\rho}_{\text{gG}}^S$ by (66) and for those t , $\text{GAP}_{\hat{\rho}_{\Psi_t}^S} \approx \text{GAP}_{\hat{\rho}_{\text{gG}}^S}$ by (99), we obtain (130), as claimed.

A Proof of Remark 2

We first show that if we had chosen F differently, it would not have changed $\hat{\rho}_{\text{gG}}$. Indeed, any other $\tilde{F}$ would have been of the form $\tilde{F} = GF$ with $G : \mathbb{R}^{K-1} \rightarrow \mathbb{R}^{K-1}$ an invertible linear mapping, so that (with $\lambda = (\lambda_1, \dots, \lambda_{K-1})$ and $\cdot$ the dot product in $\mathbb{R}^{K-1}$)

$$\sum_{k=0}^{K-1} \lambda_k F_k(\hat{N}_1, \dots, \hat{N}_r) = \lambda \cdot F(\hat{N}_1, \dots, \hat{N}_r) \quad (131)$$

$$= ((G^{-1})^\dagger \lambda) \cdot (GF(\hat{N}_1, \dots, \hat{N}_r)) \quad (132)$$

$$= \tilde{\lambda} \cdot \tilde{F}(\hat{N}_1, \dots, \hat{N}_r) \quad (133)$$

with

$$\tilde{\lambda} = (G^{-1})^\dagger \lambda. \quad (134)$$

Thus, $\tilde{\rho}_{\text{gG}}$ obtained from $\tilde{F}$ and $\tilde{\lambda}$ coincides with $\hat{\rho}_{\text{gG}}$ obtained from F and λ ; it remains to check that the λ values obtained from $\tilde{F}$ agree with $\tilde{\lambda}$. Since $\tilde{Q}_k = \tilde{F}_k(\hat{N}_1, \dots, \hat{N}_r) = G_k(\hat{Q}_1, \dots, \hat{Q}_{K-1})$ and $\tilde{Q}_k = G_k(Q_1, \dots, Q_{K-1})$, we obtain from (10) for $k = 1, \dots, K-1$ by applying the linear mapping G on both sides that $\text{tr}(\tilde{\rho}_{\text{gG}} \tilde{Q}_k) = \tilde{Q}_k$, which completes the proof.

Now we show that if we had chosen F differently, it would have changed $\hat{\rho}_{\text{gmc}}$. Indeed, the axiparallel rectangle $\prod_{k=1}^{K-1} [Q_k - \Delta Q_k, Q_k]$ would be mapped by G to a parallelepiped instead of the axiparallel rectangle $\prod_{k=1}^{K-1} [\tilde{Q}_k - \Delta \tilde{Q}_k, \tilde{Q}_k]$ with the same corner $(\tilde{Q}_1, \dots, \tilde{Q}_{K-1})$. If the density of states (jointly for $\hat{Q}_1, \dots, \hat{Q}_K$) grows quickly with each variable, most joint eigenvalues in either set are expected to lie close to that corner, but still the opening angle at that corner would be different.

B Proof of Remark 3

If $\tilde{E}_{01}, \dots, \tilde{E}_{0r}$ solve (21) as well, then $\mathcal{E} := (\tilde{E}_{01} - E_{01}, \dots, \tilde{E}_{0r} - E_{0r})$ is orthogonal to $\mathcal{L}$; $\hat{H}$ gets changed to $\tilde{\hat{H}} = \hat{H} + \sum_i \mathcal{E}_i \hat{N}_i$, analogously $\hat{H}_0$, and E to $\tilde{E} = E + \sum_i \mathcal{E}_i n_{0i}$. (For the purpose of this consideration, we may imagine a second set of molecules $\tilde{A}_i$ subject to reactions exactly analogous to (14) but with different ground state energies $\tilde{E}_{0i}$; in practice, $\tilde{\hat{H}}$ may be our guess at the correct Hamiltonian.) Since $(n_{\text{eq},1} - n_{01}, \dots, n_{\text{eq},r} - n_{0r}) \in \mathcal{L}$ and $\mathcal{E} \perp \mathcal{L}$, also $\tilde{E} = E + \sum_i \mathcal{E}_i n_{\text{eq},i}$. At the same time, $F, \tilde{Q}_k$, and Q_k ($k \leq K-1$) do not change. It follows that the choices $\tilde{\beta} = \beta$ and $\tilde{\mu}_{0i} = \mu_{0i} - \mathcal{E}_i$ will lead to $\tilde{\rho}_{\text{gG}} = \hat{\rho}_{\text{gG}} = \hat{\rho}_{\text{gc}} = \tilde{\rho}_{\text{gc}}$ and thus satisfy (10) with $\tilde{Q}_k = Q_k$ ($k \leq K-1$) and $\tilde{Q}_K = \tilde{E}$ on the right-hand side and $\tilde{Q}_K = \tilde{\hat{H}}$ included on the left. Furthermore, $\tilde{\mu}_{0i}$ and $\tilde{E}_{0i}$ satisfy (35); since the correct values of $\tilde{\beta}$ and $\tilde{\mu}_{0i}$ are determined by (10) and (35), this confirms that $\tilde{\beta} = \beta$ and $\tilde{\mu}_{0i} = \mu_{0i} - \mathcal{E}_i$, so $\hat{\rho}_{\text{gc}}$ stays the same. Moreover, $\hat{\rho}_{\text{gmc}}$ stays the same under the condition stated in Remark 3 because $\mathcal{H}_{\text{gmc}}$ stays the same (if we neglect $\hat{V}$) because, put briefly, any change of particle numbers within $\mathcal{H}_{\text{gmc}}$ lies in $\mathcal{L}$ while $\mathcal{E} \perp \mathcal{L}$.

C Proof of Example 1

Lemma 1. *Let $M \in \mathbb{N}$. The function $\varrho(q) = C 1_{0 < q < Q} q^M$ is a probability density for $C = (M+1)/Q^{M+1}$ and has standard deviation $\sigma = Q\sqrt{M+1}/(M+2)\sqrt{M+3}$ (asymptotically Q/M as $M \rightarrow \infty$). The function $\tilde{\varrho}(q) = \tilde{C}_M 1_{0 < q} q^M e^{-\lambda q}$ is a probability density for $\lambda > 0$ and $\tilde{C}_M = M!/\lambda^{M+1}$, has expectation Q for $\lambda = (M+1)/Q$, and has standard deviation $\tilde{\sigma} = Q/\sqrt{M+1}$ (asymptotically $Q/\sqrt{M}$ as $M \rightarrow \infty$).*

Proof. This is a straightforward calculation that we include for the convenience of the reader. The value of C is determined by

$$1 = \int_0^Q dq C q^M = C \frac{Q^{M+1}}{M+1}. \quad (135)$$

The mean of ϱ is

$$\langle q \rangle_{\varrho} = \int_0^Q dq \frac{M+1}{Q^{M+1}} q^{M+1} = \frac{(M+1)Q^{M+2}}{Q^{M+1}(M+2)} = \frac{M+1}{M+2}Q, \quad (136)$$

the second moment

$$\langle q^2 \rangle_{\varrho} = \int_0^Q dq \frac{M+1}{Q^{M+1}} q^{M+2} = \frac{M+1}{M+3}Q^2. \quad (137)$$

Thus, the variance is

$$\text{Var}_{\varrho} = \langle q^2 \rangle_{\varrho} - \langle q \rangle_{\varrho}^2 \quad (138a)$$

$$= Q^2 \left[\frac{M+1}{M+3} - \left(\frac{M+1}{M+2} \right)^2 \right] \quad (138b)$$

$$= Q^2 \frac{M+1}{(M+3)(M+2)^2}, \quad (138c)$$

which yields the standard deviation σ in the lemma.

We turn to $\tilde{q}$:

$$\frac{1}{\tilde{C}_M} = \int_0^\infty dq q^M \exp(-\lambda q) \quad (139a)$$

$$= \left[-q^M \exp(-\lambda q) / \lambda \right]_0^\infty + \frac{M}{\lambda} \int_0^\infty dq q^{M-1} \exp(-\lambda q) \quad (139b)$$

$$= \frac{M}{\lambda} \int_0^\infty dq q^{M-1} \exp(-\lambda q) = \dots = \quad (139c)$$

$$= \frac{M!}{\lambda^{M+1}}. \quad (139d)$$

The mean of $\tilde{q}$ is

$$\langle q \rangle_{\tilde{q}} = \int_0^\infty dq \tilde{C}_M q^{M+1} \exp(-\lambda q) \quad (140a)$$

$$= \frac{\tilde{C}_M}{\tilde{C}_{M+1}} = \frac{\lambda^{M+1}(M+1)!}{M!\lambda^{M+2}} = \frac{M+1}{\lambda}. \quad (140b)$$

Setting it equal to Q yields $\lambda = (M+1)/Q$. The second moment is

$$\langle q^2 \rangle_{\tilde{q}} = \int_0^\infty dq \tilde{C}_M q^{M+2} \exp(-\lambda q) \quad (141a)$$

$$= \frac{\tilde{C}_M}{\tilde{C}_{M+2}} = \frac{\lambda^{M+1}(M+2)!}{M!\lambda^{M+3}} = \frac{(M+1)(M+2)}{\lambda^2} = \frac{M+2}{M+1} Q^2. \quad (141b)$$

Thus, the variance is

$$\text{Var}_{\tilde{q}} = \langle q^2 \rangle_{\tilde{q}} - \langle q \rangle_{\tilde{q}}^2 \quad (142a)$$

$$= \frac{M+2}{M+1} Q^2 - Q^2 = \frac{Q^2}{M+1}, \quad (142b)$$

which yields the standard deviation $\tilde{\sigma}$ mentioned in the lemma. $\square$

D Proof of Proposition 1

Existence: By (85),

$$\hat{I}^a \otimes \hat{Q}^{bc} - \hat{I}^a \otimes \hat{I}^b \otimes \hat{Q}^c = \hat{Q}^{ab} \otimes \hat{I}^c - \hat{Q}^a \otimes \hat{I}^b \otimes \hat{I}^c. \quad (143)$$

Since the left-hand side is of the form $\hat{I}^a \otimes \hat{R}^{bc}$ and the right-hand side of the form $\hat{R}^{ab} \otimes \hat{I}^c$, both sides have to be of the form $\hat{I}^a \otimes \hat{Q}^b \otimes \hat{I}^c$. For the left-hand side, it follows (after dropping a factor $\hat{I}^a$) that $\hat{Q}^{bc} = \hat{Q}^b \otimes \hat{I}^c + \hat{I}^b \otimes \hat{Q}^c$. For the right-hand side, it follows (after dropping a factor $\hat{I}^c$) that $\hat{Q}^{ab} = \hat{Q}^a \otimes \hat{I}^b + \hat{I}^a \otimes \hat{Q}^b$, as claimed.

Uniqueness: Insert (86a) into (85), so $\hat{I}^a \otimes \hat{I}^b \otimes \hat{Q}^c$ cancels out; drop the common factor $\hat{I}^c$ and take the partial trace over $\mathcal{H}^a$ to obtain that $\hat{Q}^b = (\dim \mathcal{H}^a)^{-1} (\text{tr}^a \hat{Q}^{ab} - (\text{tr} \hat{Q}^a) \hat{I}^b)$.

E Proof of Proposition 2

Let $\hat{\Pi}_e$ denote the projection to the eigenspace of $\hat{H}$ with eigenvalue $e \in \mathcal{E}$. We first show that for all $\psi_0 \in \mathbb{S}(\mathcal{H}_R)$, the time average (defined in general as in (127)) of $\text{tr}^B |\psi_t\rangle\langle\psi_t|$ is close to $\text{tr}^B \hat{\rho}_R$. Since $\psi_t = \sum_{e \in \mathcal{E}} e^{-iet} \hat{\Pi}_e \psi_0$, the time average of $\text{tr}^B |\psi_t\rangle\langle\psi_t|$ is given by

$$\overline{\text{tr}^B |\psi_t\rangle\langle\psi_t|} = \text{tr}^B \sum_{e, e' \in \mathcal{E}} \overline{e^{i(e-e')t}} \hat{\Pi}_{e'} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e \quad (144a)$$

$$= \sum_{e \in \mathcal{E}} \text{tr}^B \hat{\Pi}_e |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e. \quad (144b)$$

Without loss of generality we assume that $\hat{\Pi}_e \psi_0 \neq 0$ for all e . Since $\hat{H}$ and $\hat{P}_R$ are simultaneously diagonalizable, $\hat{\Pi}_e \psi_0 \in \mathcal{H}_R$; thus, since $\phi_1 := \hat{\Pi}_e \psi_0 / \|\hat{\Pi}_e \psi_0\|$ is an eigenvector, (123) implies that

$$\left\| \overline{\text{tr}^B |\psi_t\rangle\langle\psi_t|} - \text{tr}^B \hat{\rho}_R \right\|_2 = \left\| \sum_{e \in \mathcal{E}} \|\hat{\Pi}_e \psi_0\|^2 \left(\text{tr}^B \frac{\hat{\Pi}_e |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e}{\|\hat{\Pi}_e \psi_0\|^2} - \text{tr}^B \hat{\rho}_R \right) \right\|_2 \quad (145a)$$

$$\leq \sum_{e \in \mathcal{E}} \|\hat{\Pi}_e \psi_0\|^2 \left\| \text{tr}^B \frac{\hat{\Pi}_e |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e}{\|\hat{\Pi}_e \psi_0\|^2} - \text{tr}^B \hat{\rho}_R \right\|_2 \quad (145b)$$

$$< \sum_{e \in \mathcal{E}} \|\hat{\Pi}_e \psi_0\|^2 \varepsilon \quad (145c)$$

$$= \varepsilon. \quad (145d)$$

Next we show that the time variance of $\text{tr}^B |\psi_t\rangle\langle\psi_t|$ is small. To this end we compute (with the notation $|\hat{A}|^2 = \hat{A} \hat{A}^\dagger$)

$$\begin{aligned} & \left\| \overline{\text{tr}^B |\psi_t\rangle\langle\psi_t|} - \text{tr}^B |\psi_t\rangle\langle\psi_t| \right\|_2^2 \\ &= \left\| \text{tr}^B \sum_{e, e'} e^{i(e-e')t} \hat{\Pi}_{e'} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e - \overline{\text{tr}^B |\psi_t\rangle\langle\psi_t|} \right\|_2^2 \end{aligned} \quad (146a)$$

$$= \left\| \sum_{e \neq e'} e^{i(e-e')t} \text{tr}^B \hat{\Pi}_{e'} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e \right\|_2^2 \quad (146b)$$

$$= \text{tr}^S \left| \sum_{e \neq e'} e^{i(e-e')t} \text{tr}^B \hat{\Pi}_{e'} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e \right|^2 \quad (146c)$$

$$= \text{tr}^S \sum_{\substack{e \neq e' \\ e'' \neq e'''}} \overline{e^{i(e-e'-e''+e''')t}} \left(\text{tr}^B \hat{\Pi}_{e'} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e \right) \left(\text{tr}^B \hat{\Pi}_{e'''} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_{e''} \right) \quad (146d)$$

$$= \sum_{\substack{e \neq e' \\ e'' \neq e'''}} \delta_{e-e'-e''+e''', 0} \text{tr}^S \left(\left(\text{tr}^B \hat{\Pi}_{e'} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e \right) \left(\text{tr}^B \hat{\Pi}_{e'''} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_{e''} \right) \right). \quad (146e)$$

With the help of the Cauchy-Schwarz inequality for tr^S we find that

$$\begin{aligned} & \left| \text{tr}^S \left(\left(\text{tr}^B \hat{\Pi}_{e'} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e \right) \left(\text{tr}^B \hat{\Pi}_{e'''} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_{e''} \right) \right) \right| \\ & \leq \sqrt{\text{tr}^S \left[\left(\text{tr}^B \hat{\Pi}_{e'} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e \right) \left(\text{tr}^B \hat{\Pi}_{e'} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e \right)^* \right]} \\ & \quad \cdot \sqrt{\text{tr}^S \left[\left(\text{tr}^B \hat{\Pi}_{e'''} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_{e''} \right)^* \left(\text{tr}^B \hat{\Pi}_{e'''} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_{e''} \right) \right]} \end{aligned} \quad (147a)$$

$$= \left\| \text{tr}^B \hat{\Pi}_{e'} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e \right\|_2 \left\| \text{tr}^B \hat{\Pi}_{e'''} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_{e''} \right\|_2. \quad (147b)$$

For $\alpha = (e, e') \in \mathcal{G} := \{(\tilde{e}, \tilde{e}') \in \mathcal{E} \times \mathcal{E}, \tilde{e} \neq \tilde{e}'\}$ we define $v_\alpha = \left\| \text{tr}^B \hat{\Pi}_{e'} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e \right\|_2$ and $\Delta_\alpha = e - e'$. Moreover, in a move we adopt from [45], we define the matrix R by

$$R_{\alpha\beta} := \delta_{\Delta_\alpha, \Delta_\beta}. \quad (148)$$

With this it follows that

$$\left\| \text{tr}^B |\psi_t\rangle\langle\psi_t| - \overline{\text{tr}^B |\psi_t\rangle\langle\psi_t|} \right\|_2^2 \leq \sum_{\alpha, \beta} v_\alpha^* R_{\alpha\beta} v_\beta \quad (149a)$$

$$\leq \|R\| \sum_{\alpha} |v_\alpha|^2 \quad (149b)$$

$$\leq \|R\| \sum_{e \neq e'} \left\| \text{tr}^B \hat{\Pi}_{e'} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e \right\|_2^2. \quad (149c)$$

We have that $\|R\| \leq \sqrt{\|R\|_1 \|R\|_\infty}$, where $\|R\|_1 := \max_{\|u\|_1=1} \|Ru\|_1$ with $\|u\|_1 = \sum_{\alpha} |u_\alpha|$ and $\|R\|_\infty := \max_{\|u\|_\infty=1} \|Ru\|_\infty$ with $\|u\|_\infty = \max_{\alpha} |u_\alpha|$. As R is Hermitian, $\|R\|_1 = \|R\|_\infty$, and we have the bound

$$\|R\| \leq \max_{\beta} \sum_{\alpha} |R_{\alpha\beta}| = D_G. \quad (150)$$

With this and the help of the MITE-ETH we obtain

$$\left\| \text{tr}^B |\psi_t\rangle\langle\psi_t| - \overline{\text{tr}^B |\psi_t\rangle\langle\psi_t|} \right\|_2^2 \leq D_G \sum_{e \neq e'} \|\hat{\Pi}_e \psi_0\|^2 \|\hat{\Pi}_{e'} \psi_0\|^2 \left\| \text{tr}^B \frac{\hat{\Pi}_{e'} |\psi_0\rangle\langle\psi_0| \hat{\Pi}_e}{\|\hat{\Pi}_{e'} \psi_0\| \|\hat{\Pi}_e \psi_0\|} \right\|_2^2 \quad (151a)$$

$$\leq D_G \sum_{e, e'} \|\hat{\Pi}_e \psi_0\|^2 \|\hat{\Pi}_{e'} \psi_0\|^2 \varepsilon^2 \quad (151b)$$

$$= D_G \varepsilon^2. \quad (151c)$$

Markov's inequality says that

$$\mathbb{P}(Y \geq a) \leq \mathbb{E}Y/a \quad (152)$$

for any random variable $Y \geq 0$ and $a > 0$. It implies that (with the notation $|M|$ for the length (Lebesgue measure) of the set $M \subseteq \mathbb{R}$)

$$\liminf_{T \rightarrow \infty} \frac{1}{T} \left| \left\{ t \in [0, T] : \left\| \text{tr}^B |\psi_t\rangle\langle\psi_t| - \overline{\text{tr}^B |\psi_t\rangle\langle\psi_t|} \right\|_2 > \varepsilon \sqrt{\frac{D_G}{\delta}} \right\} \right|$$

$$= \liminf_{T \rightarrow \infty} \frac{1}{T} \left| \left\{ t \in [0, T] : \left\| \text{tr}^B |\psi_t\rangle\langle\psi_t| - \overline{\text{tr}^B |\psi_t\rangle\langle\psi_t|} \right\|_2^2 > \varepsilon^2 \frac{D_G}{\delta} \right\} \right| \quad (153a)$$

$$\leq \frac{\delta}{\varepsilon^2 D_G} \left\| \text{tr}^B |\psi_t\rangle\langle\psi_t| - \overline{\text{tr}^B |\psi_t\rangle\langle\psi_t|} \right\|_2^2 \quad (153b)$$

$$\leq \delta. \quad (153c)$$

Therefore and as a consequence of the triangle inequality, every $\psi_0 \in \mathbb{S}(\mathcal{H}_R)$ is such that for $(1 - \delta)$ -most $t \in [0, \infty)$,

$$\left\| \text{tr}^B |\psi_t\rangle\langle\psi_t| - \text{tr}^B \hat{\rho}_R \right\|_2 \leq \left\| \text{tr}^B |\psi_t\rangle\langle\psi_t| - \overline{\text{tr}^B |\psi_t\rangle\langle\psi_t|} \right\|_2 + \left\| \overline{\text{tr}^B |\psi_t\rangle\langle\psi_t|} - \text{tr}^B \hat{\rho}_R \right\|_2 \quad (154a)$$

$$\leq 2\varepsilon \sqrt{\frac{D_G}{\delta}}, \quad (154b)$$

which finishes the proof.

F Proof of Proposition 3

If for any given t , $(1 - \delta_x)$ -most $x \in X$ are such that $F(x, t) \leq \varepsilon$, then, since for the exceptional x 's at least $F(x, t) \leq C$, we have for the x -average that

$$\int_X \mathbb{P}(dx) F(x, t) \leq \varepsilon + C\delta_x. \quad (155)$$

By assumption, this bound holds for $(1 - \delta_t)$ -most $t \geq 0$. Since for every t , $\int_X \mathbb{P}(dx) F(x, t) \leq C$,

$$\limsup_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \int_X \mathbb{P}(dx) F(x, t) \leq \varepsilon + C\delta_x + C\delta_t. \quad (156)$$

By Tonelli's or Fubini's theorem, we can change the order of integration:

$$\limsup_{T \rightarrow \infty} \int_X \mathbb{P}(dx) \frac{1}{T} \int_0^T dt F(x, t) \leq \varepsilon + C\delta_x + C\delta_t. \quad (157)$$

We now use assumption (127); since the limit has to lie in $[0, C]$, we can apply the dominated convergence theorem (with dominating function of x given by the constant C), so we can interchange the limit and the x -integral and obtain that

$$\int_X \mathbb{P}(dx) \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt F(x, t) = \lim_{T \rightarrow \infty} \int_X \mathbb{P}(dx) \frac{1}{T} \int_0^T dt F(x, t) \leq \varepsilon + C\delta_x + C\delta_t. \quad (158)$$

We apply Markov's inequality (152) to x : for any $\varepsilon'' > 0$ for $(1 - \delta'_x)$ -most x ,

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt F(x, t) < \varepsilon'' \quad (159)$$

with

$$\delta'_x = \frac{\varepsilon + C\delta_x + C\delta_t}{\varepsilon''}. \quad (160)$$

Fix any x for which (159) holds. By Markov's inequality applied to t , for any $\varepsilon' > 0$ for $(1 - \delta'_t)$ -most $t \geq 0$,

$$F(x, t) \leq \varepsilon' \quad (161)$$

with

$$\delta'_t = \frac{\varepsilon''}{\varepsilon'}. \quad (162)$$

Regarding ε' as given and ε'' as defined by the last equation, we obtain the conclusion of Proposition 3.

G Proof of Proposition 4

Suppose first that $\hat{H}$ has rationally independent eigenvalues (which occurs generically in the sense that it occurs with probability 1 if $\hat{H}$ is random with continuous distribution). Let (ϕ_n) be an eigen-ONB of $\hat{H} = \sum_n e_n |\phi_n\rangle\langle\phi_n|$ and expand $\Psi = \sum_n c_n \phi_n$ in this basis, so $\Psi_t = \sum_n e^{-ie_n t} c_n \phi_n$. Then it is known [59, 57] that the dynamics of Ψ_t is ergodic on the torus $\mathcal{T} := \{\Phi \in \mathcal{H} : |\langle\phi_n|\Phi\rangle| = |c_n|\}$ defined by the moduli of the energy coefficients. Therefore, for any bounded measurable g and almost every Ψ_0 , the time average of $g(\Psi_t)$ is equal to the phase average. Since the torus is compact and g bounded, the phase average exists, so also the time average exists. In fact, since the dynamics is quasi-periodic, the time average exists for *every* (rather than *almost every*) Ψ_0 .

But even if the eigenvalues of $\hat{H}$ are not rationally independent, so certain phase relations become periodic rather than quasi-periodic and the dynamics is not ergodic on $\mathcal{T}$, the dynamics is still ergodic on a lower-dimensional submanifold $\mathcal{S}$, and again the time average exists and equals the phase average over $\mathcal{S}$. This completes the proof of Proposition 4.

An alternative strategy of proof, at least for almost every Ψ_0 , is based on the theorem [41, 42] that a measure-preserving dynamical system with finite measure on a Lebesgue space can be decomposed into ergodic components. For ergodic systems for almost every initial condition, the time average of any bounded measurable function exists and is equal to the phase average. Thus, for almost every initial condition the time average exists. Since a Hilbert space is a complete metric space and thus a Lebesgue space, and since in finite dimension $u_{\mathbb{S}(\mathcal{H})}$ is finite and preserved, the dynamical system of Proposition 4 is contained as a special case.

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