On the Distribution of the Wave Function for Systems in Thermal Equilibrium

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Abstract

For a quantum system, a density matrix ρ that is not pure can arise, via averaging, from a distribution μ of its wave function, a normalized vector belonging to its Hilbert space $\mathscr{H}$. While ρ itself does not determine a unique μ, additional facts, such as that the system has come to thermal equilibrium, might. It is thus not unreasonable to ask, which μ, if any, corresponds to a given thermodynamic ensemble? To answer this question we construct, for any given density matrix ρ, a natural measure on the unit sphere in $\mathscr{H}$, denoted $GAP(\rho)$. We do this using a suitable projection of the Gaussian measure on $\mathscr{H}$ with covariance ρ. We establish some nice properties of $GAP(\rho)$ and show that this measure arises naturally when considering macroscopic systems. In particular, we argue that it is the most appropriate choice for systems in thermal equilibrium, described by the canonical ensemble density matrix $\rho_\beta = (1/Z)\exp(-\beta H)$. $GAP(\rho)$ may also be relevant to quantum chaos and to the stochastic evolution of open quantum systems, where distributions on $\mathscr{H}$ are often used.

Key words: canonical ensemble in quantum theory; probability measures on Hilbert space; Gaussian measures; density matrices.

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1 Introduction

In classical mechanics, ensembles, such as the microcanonical and canonical ensembles, are represented by probability distributions on the phase space. In quantum mechanics, ensembles are usually represented by density matrices. It is natural to regard these density matrices as arising from probability distributions on the (normalized) wave functions associated with the thermodynamical ensembles, so that members of the ensemble are represented by a random state vector. There are, however, as is well known, many probability distributions which give rise to the same density matrix, and thus to the same predictions for experimental outcomes [25, sec. IV.3].[1] Moreover, as emphasized by Landau and Lifshitz [13, sec. I.5], the energy levels for macroscopic systems are so closely spaced (exponentially small in the number of particles in the system) that "the concept of stationary states [energy eigenfunctions] becomes in a certain sense unrealistic" because of the difficulty of preparing a system with such a sharp energy and keeping it isolated. Landau and Lifshitz are therefore wary of, and warn against, regarding the density matrix for such a system as arising solely from our lack of knowledge about the wave function of the system. We shall argue, however, that despite these caveats such distributions can be both useful and physically meaningful. In particular we describe here a novel probability distribution, to be associated with any thermal ensemble such as the canonical ensemble.

While probability distributions on wave functions are natural objects of study in many contexts, from quantum chaos [3, 12, 23] to open quantum systems [4], our main motivation for considering them is to exploit the analogy between classical and quantum statistical mechanics [20, 21, 26, 14, 15, 16]. This analogy suggests that some relevant classical reasonings can be transferred to quantum mechanics by formally replacing the classical phase space by the unit sphere $\mathscr{S}(\mathscr{H})$ of the quantum system's Hilbert space $\mathscr{H}$. In particular, with a natural measure $\mu(d\psi)$ on $\mathscr{S}(\mathscr{H})$ one can utilize the notion of typicality, i.e., consider properties of a system common to "almost all" members of an ensemble. This is a notion frequently used in equilibrium statistical mechanics, as in, e.g., Boltzmann's recognition that typical phase points on the energy surface of a macroscopic system are such that the empirical distribution of velocities is approximately Maxwellian. Once one has such a measure for quantum systems, one could attempt an analysis of the second law of thermodynamics in quantum mechanics along the lines of

[1] This empirical equivalence should not too hastily be regarded as implying physical equivalence. Consider, for example, the two Schrödinger's cat states $\Psi_\pm = (\Psi_{\text{alive}} \pm \Psi_{\text{dead}})/\sqrt{2}$. The measure that gives equal weight to these two states corresponds to the same density matrix as the one giving equal weight to Ψ_{alive} and Ψ_{dead}. However the physical situation corresponding to the former measure, a mixture of two grotesque superpositions, seems dramatically different from the one corresponding to the latter, a routine mixture. It is thus not easy to regard these two measures as physically equivalent.

Boltzmann's analysis of the second law in classical mechanics, involving an argument to the effect that the behavior described in the second law (such as entropy increase) occurs for typical states of an isolated macroscopic system, i.e. for the overwhelming majority of points on $\mathscr{S}(\mathscr{H})$ with respect to $\mu(d\psi)$.

Probability distributions on wave functions of a composite system, with Hilbert space $\mathscr{H}$, have in fact been used to establish the typical properties of the reduced density matrix of a subsystem arising from the wave function of the composite. For example, Page [19] considers the uniform distribution on $\mathscr{S}(\mathscr{H})$ for a finite-dimensional Hilbert space $\mathscr{H}$, in terms of which he shows that the von Neumann entropy of the reduced density matrix is typically nearly maximal under appropriate conditions on the dimensions of the relevant Hilbert spaces.

Given a probability distribution μ on the unit sphere $\mathscr{S}(\mathscr{H})$ of the Hilbert space $\mathscr{H}$ there is always an associated density matrix ρ_μ [25]: it is the density matrix of the mixture, or the statistical ensemble of systems, defined by the distribution μ, given by

$$\rho_\mu = \int\limits_{\mathscr{S}(\mathscr{H})} \mu(d\psi)\, |\psi\rangle\langle\psi| \,. \tag{1}$$

For any projection operator P, $\mathrm{tr}\,(\rho_\mu P)$ is the probability of obtaining in an experiment a result corresponding to P for a system with a μ-distributed wave function. It is evident from (1) that ρ_μ is the second moment, or covariance matrix, of μ, provided μ has mean 0 (which may, and will, be assumed without loss of generality since ψ and $-\psi$ are equivalent physically).

While a probability measure μ on $\mathscr{S}(\mathscr{H})$ determines a unique density matrix ρ on $\mathscr{H}$ via (1), the converse is not true: the association $\mu \mapsto \rho_\mu$ given by (1) is many-to-one.[2] There is furthermore no unique "physically correct" choice of μ for a given ρ since for any μ corresponding to ρ one could, in principle, prepare an ensemble of systems with wave functions distributed according to this μ. However, while ρ itself need not determine a unique probability measure, additional facts about a system, such as that it has come to thermal equilibrium, might. It is thus not unreasonable to ask: which measure on $\mathscr{S}(\mathscr{H})$ corresponds to a given thermodynamic ensemble?

Let us start with the *microcanonical* ensemble, corresponding to the energy interval $[E, E+\delta]$, where δ is small on the macroscopic scale but large enough for the interval

[2]For example, in a k-dimensional Hilbert space the uniform probability distribution $u = u_{\mathscr{S}(\mathscr{H})}$ over the unit sphere has density matrix $\rho_u = \frac{1}{k}I$ with I the identity operator on $\mathscr{H}$; at the same time, for every orthonormal basis of $\mathscr{H}$ the uniform distribution over the basis (which is a measure concentrated on just k points) has the same density matrix, $\rho = \frac{1}{k}I$. An exceptional case is the density matrix corresponding to a pure state, $\rho = |\psi\rangle\langle\psi|$, as the measure μ with this density matrix is almost unique: it must be concentrated on the ray through ψ, and thus the only non-uniqueness corresponds to the distribution of the phase.

to contain many eigenvalues. To this there is associated the spectral subspace $\mathscr{H}_{E,\delta}$, the span of the eigenstates $|n\rangle$ of the Hamiltonian H corresponding to eigenvalues E_n between E and $E+\delta$. Since $\mathscr{H}_{E,\delta}$ is finite dimensional, one can form the *microcanonical density matrix*

$$\rho_{E,\delta} = (\dim \mathscr{H}_{E,\delta})^{-1} P_{\mathscr{H}_{E,\delta}} \tag{2}$$

with $P_{\mathscr{H}_{E,\delta}} = 1_{[E,E+\delta]}(H)$ the projection to $\mathscr{H}_{E,\delta}$. This density matrix is diagonal in the energy representation and gives equal weight to all energy eigenstates in the interval $[E, E+\delta]$.

But what is the corresponding *microcanonical measure*? The most plausible answer, given long ago by Schrödinger [20, 21] and Bloch [26], is the (normalized) uniform measure $u_{E,\delta} = u_{\mathscr{S}(\mathscr{H}_{E,\delta})}$ on the unit sphere in this subspace. $\rho_{E,\delta}$ is associated with $u_{E,\delta}$ via (1).

Note that a wave function Ψ chosen at random from this distribution is almost certainly a nontrivial superposition of the eigenstates $|n\rangle$ with random coefficients $\langle n|\Psi\rangle$ that are identically distributed, but not independent. The measure $u_{E,\delta}$ is clearly stationary, i.e., invariant under the unitary time evolution generated by H, and it is as spread out as it could be over the set $\mathscr{S}(\mathscr{H}_{E,\delta})$ of allowed wave functions. This measure provides us with a notion of a "typical wave function" from $\mathscr{H}_{E,\delta}$ which is very different from the one arising from the measure $\mu_{E,\delta}$ that, when H is nondegenerate, gives equal probability $(\dim \mathscr{H}_{E,\delta})^{-1}$ to every eigenstate $|n\rangle$ with eigenvalue $E_n \in [E, E+\delta]$. The measure $\mu_{E,\delta}$, which is concentrated on these eigenstates, is, however, less robust to small perturbations in H than is the smoother measure $u_{E,\delta}$.

Our proposal for the canonical ensemble is in the spirit of the uniform microcanonical measure $u_{E,\delta}$ and reduces to it in the appropriate cases. It is based on a mathematically natural family of probability measures μ on $\mathscr{S}(\mathscr{H})$. For every density matrix ρ on $\mathscr{H}$, there is a unique member μ of this family, satisfying (1) for $\rho_\mu = \rho$, namely the *Gaussian adjusted projected measure* $GAP(\rho)$, constructed roughly as follows: Eq. (1) (i.e., the fact that ρ_μ is the covariance of μ) suggests that we start by considering the Gaussian measure $G(\rho)$ with covariance ρ (and mean 0), which could, in finitely many dimensions, be expressed by $G(\rho)(d\psi) \propto \exp(-\langle\psi|\rho^{-1}|\psi\rangle)\, d\psi$ (where $d\psi$ is the obvious Lebesgue measure on $\mathscr{H}$).[3] This is not adequate, however, since the measure that we seek must live on the sphere $\mathscr{S}(\mathscr{H})$ whereas $G(\rho)$ is spread out over all of $\mathscr{H}$. We thus adjust and then project $G(\rho)$ to $\mathscr{S}(\mathscr{H})$, in the manner described in Section 2, in order to obtain the measure $GAP(\rho)$, having the prescribed covariance ρ as well as

[3] Berry [3] has conjectured, and for some cases proven, that such measures describe interesting universal properties of chaotic energy eigenfunctions in the semiclassical regime, see also [12, 23]. It is perhaps worth considering the possibility that the GAP measures described here provide somewhat better candidates for this purpose.

other desirable properties.

It is our contention that *a quantum system in thermal equilibrium at inverse temperature β should be described by a random state vector whose distribution is given by the measure $GAP(\rho_\beta)$ associated with the density matrix for the canonical ensemble,*

$$\rho_\beta = \rho_{\mathscr{H},H,\beta} = \frac{1}{Z}\exp(-\beta H) \text{ with } Z := \text{tr}\, \exp(-\beta H). \tag{3}$$

In order to convey the significance of $GAP(\rho)$ as well as the plausibility of our proposal that $GAP(\rho_\beta)$ describes thermal equilibrium, we recall that a system described by a canonical ensemble is usually regarded as a subsystem of a larger system. It is therefore important to consider the notion of the distribution of the wave function of a subsystem. Consider a composite system in a pure state $\psi \in \mathscr{H}_1 \otimes \mathscr{H}_2$, and ask what might be meant by the wave function of the subsystem with Hilbert space $\mathscr{H}_1$. For this we propose the following. Let $\{|q_2\rangle\}$ be a (generalized) orthonormal basis of $\mathscr{H}_2$ (playing the role, say, of the eigenbasis of the position representation). For each choice of $|q_2\rangle$, the (partial) scalar product $\langle q_2|\psi\rangle$, taken in $\mathscr{H}_2$, is a vector belonging to $\mathscr{H}_1$. Regarding $|q_2\rangle$ as random, we are led to consider the random vector $\Psi_1 \in \mathscr{H}_1$ given by

$$\Psi_1 = \mathcal{N}\, \langle Q_2|\psi\rangle \tag{4}$$

where $\mathcal{N} = \mathcal{N}(\psi, Q_2) = \big\|\langle Q_2|\psi\rangle\big\|^{-1}$ is the normalizing factor and $|Q_2\rangle$ is a random element of the basis $\{|q_2\rangle\}$, chosen with the quantum distribution

$$\mathbb{P}(Q_2 = q_2) = \big\|\langle q_2|\psi\rangle\big\|^2. \tag{5}$$

We refer to Ψ_1 as the *conditional wave function* [6] of system 1. Note that Ψ_1 becomes doubly random when we start with a random wave function in $\mathscr{H}_1 \otimes \mathscr{H}_2$ instead of a fixed one.

The distribution of Ψ_1 corresponding to (4) and (5) is given by the probability measure on $\mathscr{S}(\mathscr{H}_1)$,

$$\mu_1(d\psi_1) = \mathbb{P}(\Psi_1 \in d\psi_1) = \sum_{q_2} \big\|\langle q_2|\psi\rangle\big\|^2\, \delta\big(\psi_1 - \mathcal{N}(\psi,q_2)\, \langle q_2|\psi\rangle\big)\, d\psi_1\,, \tag{6}$$

where $\delta(\psi - \phi)\, d\psi$ denotes the "delta" measure concentrated at ϕ. While the density matrix ρ_{μ_1} associated with μ_1 always equals the reduced density matrix ρ_1^{red} of system 1, given by

$$\rho_1^{\text{red}} = \text{tr}_2|\psi\rangle\langle\psi| = \sum_{q_2} \langle q_2|\psi\rangle\langle\psi|q_2\rangle\,, \tag{7}$$

the measure μ_1 itself usually depends on the choice of the basis $\{|q_2\rangle\}$. It turns out, nevertheless, as we point out in Section 5.1, that $\mu_1(d\psi_1)$ is a universal function of ρ_1^{red}

in the special case that system 2 is large and ψ is typical (with respect to the uniform distribution on all wave functions with the same reduced density matrix), namely $GAP(\rho_1^{\mathrm{red}})$. Thus $GAP(\rho)$ has a distinguished, universal status among all probability measures on $\mathscr{S}(\mathscr{H})$ with density matrix ρ.

To further support our claim that $GAP(\rho_\beta)$ is the right measure for ρ_β, we shall regard, as is usually done, the system described by ρ_β as coupled to a (very large) heat bath. The interaction between the heat bath and the system is assumed to be (in some suitable sense) negligible. We will argue that if the wave function ψ of the combined "system plus bath" has microcanonical distribution $u_{E,\delta}$, then the distribution of the conditional wave function of the (small) system is approximately $GAP(\rho_\beta)$; see Section 4.

Indeed, a stronger statement is true. As we argue in Section 5.2, even for a typical *fixed* microcanonical wave function ψ of the composite, i.e., one typical for $u_{E,\delta}$, the conditional wave function of the system, defined in (4), is then approximately $GAP(\rho_\beta)$-distributed, for a typical basis $\{|q_2\rangle\}$. This is related to the fact that for a typical microcanonical wave function ψ of the composite the reduced density matrix for the system is approximately ρ_β [7, 21]. Note that the analogous statement in classical mechanics would be wrong: for a fixed phase point ξ of the composite, be it typical or atypical, the phase point of the system could never be random, but rather would merely be the part of ξ belonging to the system.

The remainder of this paper is organized as follows. In Section 2 we define the measure $GAP(\rho)$ and obtain several ways of writing it. In Section 3 we describe some natural mathematical properties of these measures, and suggest that these properties uniquely characterize the measures. In Section 4 we argue that $GAP(\rho_\beta)$ represents the canonical ensemble. In Section 5 we outline the proof that $GAP(\rho)$ is the distribution of the conditional wave function for *most* wave functions in $\mathscr{H}_1 \otimes \mathscr{H}_2$ with reduced density matrix ρ if system 2 is large, and show that $GAP(\rho_\beta)$ is the typical distribution of the conditional wave function arising from a fixed microcanonical wave function of a system in contact with a heat bath. In Section 6 we discuss other measures that have been or might be considered as the thermal equilibrium distribution of the wave function. Finally, in Section 7 we compute explicitly the distribution of the coefficients of a $GAP(\rho_\beta)$-distributed state vector in the simplest possible example, the two-level system.

2 Definition of $GAP(\rho)$

In this section, we define, for any given density matrix ρ on a (separable) Hilbert space $\mathscr{H}$, the Gaussian adjusted projected measure $GAP(\rho)$ on $\mathscr{S}(\mathscr{H})$. This definition makes use of two auxiliary measures, $G(\rho)$ and $GA(\rho)$, defined as follows.

$G(\rho)$ is the Gaussian measure on $\mathscr{H}$ with covariance matrix ρ (and mean 0). More explicitly, let $\{|n\rangle\}$ be an orthonormal basis of eigenvectors of ρ and p_n the corresponding eigenvalues,

$$\rho = \sum_n p_n \, |n\rangle\langle n|. \tag{8}$$

Such a basis exists because ρ has finite trace. Let Z_n be a sequence of independent complex-valued random variables having a (rotationally symmetric) Gaussian distribution in $\mathbb{C}$ with mean 0 and variance

$$\mathbb{E}|Z_n|^2 = p_n \tag{9}$$

(where $\mathbb{E}$ means expectation), i.e., $\operatorname{Re} Z_n$ and $\operatorname{Im} Z_n$ are independent real Gaussian variables with mean zero and variance $p_n/2$. We define $G(\rho)$ to be the distribution of the random vector

$$\Psi^G := \sum_n Z_n |n\rangle \, . \tag{10}$$

Note that Ψ^G is not normalized, i.e., it does not lie in $\mathscr{S}(\mathscr{H})$. In order that Ψ^G lie in $\mathscr{H}$ at all, we need that the sequence Z_n be square-summable, $\sum_n |Z_n|^2 < \infty$. That this is almost surely the case follows from the fact that $\mathbb{E}\sum_n |Z_n|^2$ is finite. In fact,

$$\mathbb{E}\sum_n |Z_n|^2 = \sum_n \mathbb{E}|Z_n|^2 = \sum_n p_n = \operatorname{tr}\rho = 1. \tag{11}$$

More generally, we observe that for any measure μ on $\mathscr{H}$ with (mean 0 and) covariance given by the trace class operator C,

$$\int_{\mathscr{H}} \mu(d\psi) \, |\psi\rangle\langle\psi| = C \, ,$$

we have that, for a random vector Ψ with distribution μ, $\mathbb{E}\|\Psi\|^2 = \operatorname{tr} C$.

It also follows that Ψ^G almost surely lies in the positive spectral subspace of ρ, the closed subspace spanned by those $|n\rangle$ with $p_n \neq 0$, or, equivalently, the orthogonal complement of the kernel of ρ; we shall call this subspace support(ρ). Note further that, since $G(\rho)$ is the Gaussian measure with covariance ρ, it does not depend (in the case of degenerate ρ) on the choice of the basis $\{|n\rangle\}$ among the eigenbases of ρ, but only on ρ.

Since we want a measure on $\mathscr{S}(\mathscr{H})$ while $G(\rho)$ is not concentrated on $\mathscr{S}(\mathscr{H})$ but rather is spread out, it would be natural to project $G(\rho)$ to $\mathscr{S}(\mathscr{H})$. However, since projecting to $\mathscr{S}(\mathscr{H})$ changes the covariance of a measure, as we will point out in detail in Section 3.1, we introduce an adjustment factor that exactly compensates for the change of covariance due to projection. We thus define the adjusted Gaussian measure $GA(\rho)$ on $\mathscr{H}$ by

$$GA(\rho)(d\psi) = \|\psi\|^2 \, G(\rho)(d\psi). \tag{12}$$

Since $\mathbb{E}\|\Psi^G\|^2 = 1$ by (11), $GA(\rho)$ is a probability measure.

Let Ψ^{GA} be a $GA(\rho)$-distributed random vector. We define $GAP(\rho)$ to be the distribution of

$$\Psi^{GAP} := \frac{\Psi^{GA}}{\|\Psi^{GA}\|} = P(\Psi^{GA}) \tag{13}$$

with P the projection to the unit sphere (i.e., the normalization of a vector),

$$P : \mathscr{H} \setminus \{0\} \to \mathscr{S}(\mathscr{H}), \quad P(\psi) = \|\psi\|^{-1}\psi. \tag{14}$$

Putting (13) differently, for a subset $B \subseteq \mathscr{S}(\mathscr{H})$,

$$GAP(\rho)(B) = GA(\rho)(\mathbb{R}^+ B) = \int\limits_{\mathbb{R}^+ B} G(\rho)(d\psi) \, \|\psi\|^2 \tag{15}$$

where $\mathbb{R}^+ B$ denotes the cone through B. More succinctly,

$$GAP(\rho) = P_*\big(GA(\rho)\big) = GA(\rho) \circ P^{-1} \, . \tag{16}$$

where P_* denotes the action of P on measures.

More generally, one can define for any measure μ on $\mathscr{H}$ the "adjust-and-project" procedure: let $A(\mu)$ be the adjusted measure $A(\mu)(d\psi) = \|\psi\|^2 \, \mu(d\psi)$; then the adjusted-and-projected measure is $P_*\big(A(\mu)\big) = A(\mu) \circ P^{-1}$, thus defining a mapping $P_* \circ A$ from the measures on $\mathscr{H}$ with $\int \mu(d\psi) \, \|\psi\|^2 = 1$ to the probability measures on $\mathscr{S}(\mathscr{H})$. We then have that $GAP(\rho) = P_*\big(A(G(\rho))\big)$.

We remark that Ψ^{GAP}, too, lies in support(ρ) almost surely, and that $P(\Psi^G)$ does *not* have distribution $GAP(\rho)$—nor covariance ρ (see Sect. 3.1).

We can be more explicit in the case that ρ has finite rank $k = \dim \text{support}(\rho)$, e.g. for finite-dimensional $\mathscr{H}$: then there exists a Lebesgue volume measure λ on support$(\rho) = \mathbb{C}^k$, and we can specify the densities of $G(\rho)$ and $GA(\rho)$,

$$\frac{dG(\rho)}{d\lambda}(\psi) = \frac{1}{\pi^k \, \det \rho_+} \exp(-\langle\psi|\rho_+^{-1}|\psi\rangle), \tag{17a}$$

$$\frac{dGA(\rho)}{d\lambda}(\psi) = \frac{\|\psi\|^2}{\pi^k \, \det \rho_+} \exp(-\langle\psi|\rho_+^{-1}|\psi\rangle), \tag{17b}$$

with ρ_+ the restriction of ρ to support(ρ). Similarly, we can express $GAP(\rho)$ relative to the $(2k-1)$–dimensional surface measure u on $\mathscr{S}(\mathrm{support}(\rho))$,

$$\frac{dGAP(\rho)}{du}(\psi) = \frac{1}{\pi^k \det \rho_+} \int_0^\infty dr\, r^{2k-1}\, r^2 \exp(-r^2 \langle\psi|\rho_+^{-1}|\psi\rangle) = \tag{18a}$$

$$= \frac{k!}{2\pi^k \det \rho_+} \langle\psi|\rho_+^{-1}|\psi\rangle^{-k-1}. \tag{18b}$$

We note that

$$GAP(\rho_{E,\delta}) = u_{E,\delta}\,, \tag{19}$$

where $\rho_{E\delta}$ is the microcanonical density matrix given in (2) and $u_{E\delta}$ is the microcanonical measure.

3 Properties of $GAP(\rho)$

In this section we prove the following properties of $GAP(\rho)$:

Property 1 *The density matrix associated with $GAP(\rho)$ in the sense of* (1) *is ρ, i.e., $\rho_{GAP(\rho)} = \rho$.*

Property 2 *The association $\rho \mapsto GAP(\rho)$ is* covariant*: For any unitary operator U on $\mathscr{H}$,*

$$U_* GAP(\rho) = GAP(U\rho U^*) \tag{20}$$

where $U^* = U^{-1}$ is the adjoint of U and U_* is the action of U on measures, $U_*\mu = \mu\circ U^{-1}$. In particular, $GAP(\rho)$ is stationary under any unitary evolution that preserves ρ.

Property 3 *If $\Psi \in \mathscr{H}_1 \otimes \mathscr{H}_2$ has distribution $GAP(\rho_1 \otimes \rho_2)$ then, for any basis $\{|q_2\rangle\}$ of $\mathscr{H}_2$, the conditional wave function Ψ_1 has distribution $GAP(\rho_1)$. ("GAP of a product density matrix has GAP marginal.")*

We will refer to the property expressed in Property 3 by saying that the family of GAP measures is *hereditary*. We note that when $\Psi \in \mathscr{H}_1 \otimes \mathscr{H}_2$ has distribution $GAP(\rho)$ and ρ is not a tensor product, the distribution of Ψ_1 need not be $GAP(\rho_1^{\mathrm{red}})$ (as we will show after the proof of Property 3).

Before establishing these properties let us formulate what they say about our candidate $GAP(\rho_\beta)$ for the canonical distribution. As a consequence of Property 1, the density matrix arising from $\mu = GAP(\rho_\beta)$ in the sense of (1) is the density matrix ρ_β. As a consequence of Property 2, $GAP(\rho_\beta)$ is stationary, i.e., invariant under the unitary time evolution generated by H. As a consequence of Property 3, if $\Psi \in \mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$ has distribution $GAP(\rho_{\mathscr{H},H,\beta})$ and systems 1 and 2 are decoupled, $H = H_1 \otimes I_2 + I_1 \otimes H_2$, where I_i is the identity on $\mathscr{H}_i$, then the conditional wave function Ψ_1 of system 1 has a distribution (in $\mathscr{H}_1$) of the same kind with the same inverse temperature β, namely $GAP(\rho_{\mathscr{H}_1,H_1,\beta})$. This fits well with our claim that $GAP(\rho_\beta)$ is the thermal equilibrium distribution since one would expect that if a system is in thermal equilibrium at inverse temperature β then so are its subsystems.

We conjecture that the family of GAP measures is the only family of measures satisfying Properties 1–3. This conjecture is formulated in detail, and established for suitably continuous families of measures, in Section 6.2.

The following lemma, proven in Section 3.3, is convenient for showing that a random wave function is GAP-distributed:

Lemma 1 *Let Ω be a measurable space, μ a probability measure on Ω, and $\Psi : \Omega \to \mathscr{H}$ a Hilbert-space-valued function. If $\Psi(\omega)$ is $G(\rho)$-distributed with respect to $\mu(d\omega)$, then $\Psi(\omega)/\|\Psi(\omega)\|$ is $GAP(\rho)$-distributed with respect to $\|\Psi(\omega)\|^2\mu(d\omega)$.*

3.1 The Density Matrix

In this subsection we establish Property 1. We then add a remark on the covariance matrix.

Proof of Property 1. From (1) we find that

$$\begin{aligned}\rho_{GAP(\rho)} &= \int\limits_{\mathscr{S}(\mathscr{H})} GAP(\rho)(d\psi)\, |\psi\rangle\langle\psi| = \mathbb{E}\Big(|\Psi^{GAP}\rangle\langle\Psi^{GAP}|\Big) = \\ &\overset{(13)}{=} \mathbb{E}\Big(\|\Psi^{GA}\|^{-2}\, |\Psi^{GA}\rangle\langle\Psi^{GA}|\Big) = \int\limits_{\mathscr{H}} GA(\rho)(d\psi)\, \|\psi\|^{-2}\, |\psi\rangle\langle\psi| = \\ &\overset{(12)}{=} \int\limits_{\mathscr{H}} G(\rho)(d\psi)\, |\psi\rangle\langle\psi| = \rho\end{aligned}$$

because $\int_{\mathscr{H}} G(\rho)(d\psi)\, |\psi\rangle\langle\psi|$ is the covariance matrix of $G(\rho)$, which is ρ. (A number above an equal sign refers to the equation used to obtain the equality.) □

Remark on the covariance matrix. The equation $\rho_{GAP(\rho)} = \rho$ can be understood as expressing that $GAP(\rho)$ and $G(\rho)$ have the same covariance. For a probability measure μ on $\mathscr{H}$ with mean 0 that need not be concentrated on $\mathscr{S}(\mathscr{H})$, the covariance matrix C_μ is given by

$$C_\mu = \int\limits_{\mathscr{H}} \mu(d\phi)\, |\phi\rangle\langle\phi|. \tag{21}$$

Suppose we want to obtain from μ a probability measure on $\mathscr{S}(\mathscr{H})$ having the same covariance. The projection $P_*\mu$ of μ to $\mathscr{S}(\mathscr{H})$, defined by $P_*\mu(B) = \mu(\mathbb{R}^+ B)$ for $B \subseteq \mathscr{S}(\mathscr{H})$, is not what we want, as it has covariance

$$C_{P_*\mu} = \int\limits_{\mathscr{S}(\mathscr{H})} P_*\mu(d\psi)\, |\psi\rangle\langle\psi| = \int\limits_{\mathscr{H}} \mu(d\phi)\, \|\phi\|^{-2}\, |\phi\rangle\langle\phi| \neq C_\mu.$$

However, $P_*\big(A(\mu)\big)$ does the job: it has the same covariance. As a consequence, a naturally distinguished measure on $\mathscr{S}(\mathscr{H})$ with given covariance is the Gaussian adjusted projected measure, the GAP measure, with the given covariance.

3.2 $GAP(\rho)$ is Covariant

We establish Property 2 and then discuss in more general terms under which conditions a measure on $\mathscr{S}(\mathscr{H})$ is stationary.

Proof of Property 2. Under a unitary transformation U, a Gaussian measure with covariance matrix C transforms into one with covariance matrix UCU^*. Since $\|U\psi\|^2 = \|\psi\|^2$, $GA(C)$ transforms into $GA(UCU^*)$; that is, $U\Psi_C^{GA}$ and $\Psi_{UCU^*}^{GA}$ are equal in distribution, and since $\|U\Psi_C^{GA}\| = \|\Psi_C^{GA}\|$, we have that $U\Psi_C^{GAP}$ and $\Psi_{UCU^*}^{GAP}$ are equal in distribution. In other words, $GAP(C)$ transforms into $GAP(UCU^*)$, which is what we claimed in (20). $\square$

3.2.1 Stationarity

In this subsection we discuss a criterion for stationarity under the evolution generated by $H = \sum_n E_n\, |n\rangle\langle n|$. Consider the following property of a sequence of complex random variables Z_n:

> The phases $Z_n/|Z_n|$, when they exist, are independent of the moduli $|Z_n|$ and of each other, and are uniformly distributed on $S^1 = \{e^{i\theta} : \theta \in \mathbb{R}\}$. (22)

(The phase $Z_n/|Z_n|$ exists when $Z_n \neq 0$.) Condition (22) implies that the distribution of the random vector $\Psi = \sum_n Z_n |n\rangle$ is stationary, since $Z_n(t) = \exp(-iE_n t/\hbar) Z_n(0)$. Note also that (22) implies that the distribution has mean 0.

We show that the $Z_n = \langle n|\Psi^{GAP}\rangle$ have property (22). To begin with, the $Z_n = \langle n|\Psi^G\rangle$ obviously have this property since they are independent Gaussian variables. Since the density of $GA(\rho)$ relative to $G(\rho)$ is a function of the moduli alone, also the $Z_n = \langle n|\Psi^{GA}\rangle$ satisfy (22). Finally, since the $|\langle n|\Psi^{GAP}\rangle|$ are functions of the $|\langle n|\Psi^{GA}\rangle|$ while the phases of the $\langle n|\Psi^{GAP}\rangle$ equal the phases of the $\langle n|\Psi^{GA}\rangle$, also the $Z_n = \langle n|\Psi^{GAP}\rangle$ satisfy (22).

We would like to add that (22) is not merely a sufficient, but also almost a necessary condition (and *morally* a necessary condition) for stationarity. Since for any Ψ, the moduli $|Z_n| = |\langle n|\Psi\rangle|$ are constants of the motion, the evolution of Ψ takes place in the (possibly infinite-dimensional) torus

$$\Big\{ \sum_n |Z_n| e^{i\theta_n} \, |n\rangle : 0 \le \theta_n < 2\pi \Big\} \cong \prod_{n:Z_n\neq 0} S^1, \tag{23}$$

contained in $\mathscr{S}(\mathscr{H})$. Independent uniform phases correspond to the uniform measure λ on $\prod_n S^1$. λ is the only stationary measure if the motion on $\prod_n S^1$ is uniquely ergodic, and this is the case whenever the spectrum $\{E_n\}$ of H is linearly independent over the rationals $\mathbb{Q}$, i.e., when every finite linear combination $\sum_n r_n E_n$ of eigenvalues with rational coefficients r_n, not all of which vanish, is nonzero, see [2, 24].

This is true of generic Hamiltonians, so that λ is generically the unique stationary distribution on the torus. But even when the spectrum of H is linearly dependent, e.g. when there are degenerate eigenvalues, and thus further stationary measures on the torus exist, these further measures should not be relevant to thermal equilibrium measures, because of their instability against perturbations of H [11, 1].

The stationary measure λ on $\prod_n S^1$ corresponds, for given moduli $|Z_n|$ or, equivalently, by setting $|Z_n| = p(E_n)^{1/2}$ for a given probability measure p on the spectrum of H, to a stationary measure λ_p on $\mathscr{S}(\mathscr{H})$ that is concentrated on the embedded torus (23). The measures λ_p are (for generic H) the extremal stationary measures, i.e., the extremal elements of the convex set of stationary measures, of which all other stationary measures are mixtures.

3.3 GAP Measures and Gaussian Measures

Lemma 1 is more or less immediate from the definition of $GAP(\rho)$. A more detailed proof looks like this:

Proof of Lemma 1. By assumption the distribution $\mu \circ \Psi^{-1}$ of Ψ with respect to μ is $G(\rho)$. Thus for the distribution of Ψ with respect to $\mu'(d\omega) = \|\Psi(\omega)\|^2 \mu(d\omega)$, we have $\mu' \circ \Psi^{-1}(d\psi) = \|\psi\|^2 \, \mu \circ \Psi^{-1}(d\psi) = \|\psi\|^2 \, G(\rho)(d\psi) = GA(\rho)(d\psi)$. Thus, $P(\Psi(\omega))$ has distribution $P_* GA(\rho) = GAP(\rho)$. $\square$

3.4 Generalized Bases

We have already remarked in the introduction that the orthonormal basis $\{|q_2\rangle\}$ of $\mathscr{H}_2$, used in the definition of the conditional wave function, could be a *generalized* basis, such as a "continuous" basis, for which it is appropriate to write

$$I_2 = \int dq_2 \, |q_2\rangle\langle q_2|$$

instead of the "discrete" notation

$$I_2 = \sum_{q_2} |q_2\rangle\langle q_2|$$

we used in (4)–(7).

We wish to elucidate this further. A generalized orthonormal basis $\{|q_2\rangle : q_2 \in \mathcal{Q}_2\}$ indexed by the set $\mathcal{Q}_2$ is mathematically defined by a unitary isomorphism $\mathscr{H}_2 \to L^2(\mathcal{Q}_2, dq_2)$, where dq_2 denotes a measure on $\mathcal{Q}_2$. We can think of $\mathcal{Q}_2$ as the configuration space of system 2; as a typical example, system 2 may consist of N_2 particles in a box $\Lambda \subset \mathbb{R}^3$, so that its configuration space is $\mathcal{Q}_2 = \Lambda^{N_2}$ with dq_2 the Lebesgue measure (which can be regarded as obtained by combining N_2 copies of the volume measure on $\mathbb{R}^3$).[4] The formal ket $|q_2\rangle$ then means the delta function centered at q_2; it is to be treated as (though strictly speaking it is not) an element of $\mathscr{H}_2$.

The definition of the conditional wave function Ψ_1 then reads as follows: The vector $\psi \in \mathscr{H}_1 \otimes \mathscr{H}_2$ can be regarded, using the isomorphism $\mathscr{H}_2 \to L^2(\mathcal{Q}_2, dq_2)$, as a function $\psi : \mathcal{Q}_2 \to \mathscr{H}_1$. Eq. (4) is to be understood as meaning

$$\Psi_1 = \mathcal{N} \, \psi(Q_2) \tag{24}$$

where

$$\mathcal{N} = \mathcal{N}(\psi, Q_2) = \big\|\psi(Q_2)\big\|^{-1}$$

is the normalizing factor and Q_2 is a random point in $\mathcal{Q}_2$, chosen with the quantum distribution

$$\mathbb{P}(Q_2 \in dq_2) = \big\|\psi(q_2)\big\|^2 dq_2 \,, \tag{25}$$

which is how (5) is to be understood in this setting. As ψ is defined only up to changes on a null set in $\mathcal{Q}_2$, Ψ_1 may not be defined for a particular Q_2. Its distribution in $\mathscr{H}_1$, however, is defined unambiguously by (24). In the most familiar setting with $\mathscr{H}_1 = L^2(\mathcal{Q}_1, dq_1)$, we have that $(\psi(Q_2))(q_1) = \psi(q_1, Q_2)$.

In the following, we will allow generalized bases and use continuous instead of discrete notation, and set $\langle Q_2|\psi\rangle = \psi(Q_2)$.

[4] In fact, in the original definition of the conditional wave function in [6], q_2 was supposed to be the *configuration*, corresponding to the positions of the particles belonging to system 2. For our purposes here, however, the physical meaning of the q_2 is irrelevant, so that any generalized orthonormal basis of $\mathscr{H}_2$ can be used.

3.5 Distribution of the Wave Function of a Subsystem

Proof of Property 3. The proof is divided into four steps.

Step 1. We can assume that $\Psi = P(\Psi^{GA})$ where Ψ^{GA} is a $GA(\rho)$-distributed random vector in $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$. We then have that $\Psi_1 = P_1\big(\langle Q_2|\Psi\rangle\big) = P_1\big(\langle Q_2|\Psi^{GA}\rangle\big)$ where P_1 is the normalization in $\mathscr{H}_1$, and where the distribution of Q_2, given Ψ^{GA}, is

$$\mathbb{P}(Q_2 \in dq_2|\Psi^{GA}) = \frac{\|\langle q_2|\Psi^{GA}\rangle\|^2}{\|\Psi^{GA}\|^2} dq_2 \,.$$

Ψ^{GA} and Q_2 have a joint distribution given by the following measure ν on $\mathscr{H} \times \mathcal{Q}_2$:

$$\nu(d\psi \times dq_2) = \|\langle q_2|\psi\rangle\|^2 \, G(\rho)(d\psi)\, dq_2 \,. \tag{26}$$

Thus, what needs to be shown is that with respect to ν, $P_1(\langle q_2|\psi\rangle)$ is $GAP(\rho_1)$-distributed.

Step 2. If $\Psi \in \mathscr{H}_1 \otimes \mathscr{H}_2$ is $G(\rho_1 \otimes \rho_2)$-distributed and $q_2 \in \mathcal{Q}_2$ is fixed, then the random vector $f(q_2)\,\langle q_2|\Psi\rangle \in \mathscr{H}_1$ with $f(q_2) = \langle q_2|\rho_2|q_2\rangle^{-1/2}$ is $G(\rho_1)$-distributed. This follows, more or less, from the fact that a subset of a set of jointly Gaussian random variables is also jointly Gaussian, together with the observation that the covariance of $\langle q_2|\Psi\rangle$ is

$$\int_{\mathscr{H}} G(\rho_1 \otimes \rho_1)(d\psi)\, \langle q_2|\psi\rangle\langle\psi|q_2\rangle = \langle q_2|\rho_1 \otimes \rho_2|q_2\rangle = \rho_1 \, \langle q_2|\rho_2|q_2\rangle \,.$$

More explicitly, pick an orthonormal basis $\{|n_i\rangle\}$ of $\mathscr{H}_i$ consisting of eigenvectors of ρ_i with eigenvalues $p^{(i)}_{n_i}$, and note that the vectors $|n_1, n_2\rangle := |n_1\rangle \otimes |n_2\rangle$ form an orthonormal basis of $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$ consisting of eigenvectors of $\rho_1 \otimes \rho_2$ with eigenvalues $p_{n_1,n_2} = p^{(1)}_{n_1} p^{(2)}_{n_2}$. Since the random variables $Z_{n_1,n_2} := \langle n_1, n_2|\Psi\rangle$ are independent Gaussian random variables with mean zero and variances $\mathbb{E}|Z_{n_1}, n_2|^2 = p_{n_1,n_2}$, so are their linear combinations

$$Z_{(1)n_1} := \langle n_1|f(q_2)\,\Psi(q_2)\rangle = f(q_2) \sum_{n_2} \langle q_2|n_2\rangle \, Z_{n_1,n_2}$$

with variances (because variances add when adding independent Gaussian random variables)

$$\mathbb{E}|Z_{(1)n_1}|^2 = f^2(q_2) \sum_{n_2} \big|\langle q_2|n_2\rangle\big|^2 \mathbb{E}|Z_{n_1,n_2}|^2 = p^{(1)}_{n_1} \frac{\sum_{n_2} |\langle q_2|n_2\rangle|^2 \, p^{(2)}_{n_2}}{\langle q_2|\rho_2|q_2\rangle} = p^{(1)}_{n_1}.$$

Thus $f(q_2)\,\langle q_2|\Psi\rangle$ is $G(\rho_1)$-distributed, which completes step 2.

Step 3. If $\Psi \in \mathscr{H}_1 \otimes \mathscr{H}_2$ is $G(\rho_1 \otimes \rho_2)$-distributed and $Q_2 \in \mathcal{Q}_2$ is random with any distribution, then the random vector $f(Q_2)\,\langle Q_2|\Psi\rangle$ is $G(\rho_1)$-distributed. This is a trivial consequence of step 2.

Step 4. Apply Lemma 1 as follows. Let $\Omega = \mathscr{H} \times \mathcal{Q}_2$, $\Psi(\omega) = \Psi(\psi, q_2) = f(q_2)\,\langle q_2|\psi\rangle$, and $\mu(d\psi \times dq_2) = G(\rho)(d\psi)\,\langle q_2|\rho_2|q_2\rangle\,dq_2$ (which means that q_2 and ψ are independent). By step 3, the hypothesis of Lemma 1 (for $\rho = \rho_1$) is satisfied, and thus $P_1(\Psi) = P_1(\langle q_2|\psi\rangle)$ is $GAP(\rho_1)$-distributed with respect to

$$\|\Psi(\omega)\|^2 \mu(d\omega) = f^2(q_2) \|\langle q_2|\psi\rangle\|^2\, G(\rho)(d\psi)\,\langle q_2|\rho_2|q_2\rangle\,dq_2 = \nu(d\omega)\,,$$

where we have used that $f^2(q_2) = \langle q_2|\rho_2|q_2\rangle^{-1}$. But this is, according to step 1, what we needed to show. □

To verify the statement after Property 3, consider the density matrix $\rho = |\Phi\rangle\langle\Phi|$ for a pure state Φ of the form $\Phi = \sum_n \sqrt{p_n}\,\psi_n \otimes \phi_n$, where $\{\psi_n\}$ and $\{\phi_n\}$ are respectively orthonormal bases for $\mathscr{H}_1$ and $\mathscr{H}_2$ and the p_n are nonnegative with $\sum_n p_n = 1$. Then a $GAP(\rho)$-distributed random vector Ψ coincides with Φ up to a random phase, and so $\rho_1^{\mathrm{red}} = \sum_n p_n\,|\psi_n\rangle\langle\psi_n|$. Choosing for $\{|q_2\rangle\}$ the basis $\{\phi_n\}$, the distribution of Ψ_1 is not $GAP(\rho_1^{\mathrm{red}})$ but rather is concentrated on the eigenvectors of ρ_1^{red}. When the p_n are pairwise-distinct this measure is the measure $EIG(\rho_1^{\mathrm{red}})$ we define in Section 6.1.1.

4 Microcanonical Distribution for a Large System Implies the Distribution $GAP(\rho_\beta)$ for a Subsystem

In this section we use Property 3, i.e., the fact that GAP measures are hereditary, to show that $GAP(\rho_\beta)$ is the distribution of the conditional wave function of a system coupled to a heat bath when the wave function of the composite is distributed microcanonically, i.e., according to $u_{E,\delta}$.

Consider a system with Hilbert space $\mathscr{H}_1$ coupled to a heat bath with Hilbert space $\mathscr{H}_2$. Suppose the composite system has a random wave function $\Psi \in \mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$ whose distribution is microcanonical, $u_{E,\delta}$. Assume further that the coupling is negligibly small, so that we can write for the Hamiltonian

$$H = H_1 \otimes I_2 + I_1 \otimes H_2\,, \tag{27}$$

and that the heat bath is large (so that the energy levels of H_2 are very close).

It is a well known fact that for macroscopic systems different equilibrium ensembles, for example the microcanonical and the canonical, give approximately the same answer for appropriate quantities. By this equivalence of ensembles [17], we should have that

$\rho_{E,\delta} \approx \rho_\beta$ for suitable $\beta = \beta(E)$. Then, since $GAP(\rho)$ depends continuously on ρ, we have that $u_{E,\delta} = GAP(\rho_{E,\delta}) \approx GAP(\rho_\beta)$. Thus we should have that the distribution of the conditional wave function Ψ_1 of the system is approximately the same as would be obtained when Ψ is $GAP(\rho_\beta)$-distributed. But since, by (27), the canonical density matrix is then of the form

$$\rho_\beta = \rho_{\mathscr{H},H,\beta} = \rho_{\mathscr{H}_1,H_1,\beta} \otimes \rho_{\mathscr{H}_2,H_2,\beta} \,, \tag{28}$$

we have by Property 3 that Ψ_1 is approximately $GAP(\rho_{\mathscr{H}_1,H_1,\beta})$-distributed, which is what we wanted to show.

5 Typicality of GAP Measures

The previous section concerns the distribution of the conditional wave function Ψ_1 arising from the microcanonical distribution of the wave function of the composite. It concerns, in other words, a *random* wave function of the composite. The result there is the analogue, on the level of measures on Hilbert space, of the well known result that if a microcanonical density matrix (2) is assumed for the composite, the reduced density matrix ρ_1^{red} of the system, defined as the partial trace $\mathrm{tr}_2\, \rho_{E,\delta}$, is canonical if the heat bath is large [13].

As indicated in the introduction, a stronger statement about the canonical density matrix is in fact true, namely that for a *fixed* (nonrandom) wave function ψ of the composite which is typical with respect to $u_{E,\delta}$, $\rho_1^{\mathrm{red}} \approx \rho_{\mathscr{H}_1,H_1,\beta}$ when the heat bath is large (see [7, 21]; for a rigorous study of special cases of a similar question, see [22]).[5] This stronger statement will be used in Section 5.2 to show that a similar statement holds for the distribution of Ψ_1 as well, namely that it is approximately $GAP(\rho_{\mathscr{H}_1,H_1,\beta})$-distributed for a typical fixed $\psi \in \mathscr{H}_{E,\delta}$ and basis $\{|q_2\rangle\}$ of $\mathscr{H}_2$. But we must first consider the distribution of Ψ_1 for a typical $\psi \in \mathscr{H}$.

5.1 Typicality of GAP Measures for a Subsystem of a Large System

In this section we argue that for a typical wave function of a big system the conditional wave function of a small subsystem is approximately GAP-distributed, first giving a precise formulation of this result and then sketching its proof. We give the detailed proof in [8].

[5] It is a consequence of the results in [19] that when $\dim \mathscr{H}_2 \to \infty$, the reduced density matrix becomes proportional to the identity on $\mathscr{H}_1$ for typical wave functions relative to the uniform distribution on $\mathscr{S}(\mathscr{H})$ (corresponding to $u_{E,\delta}$ for $E = 0$ and $H = 0$).

5.1.1 Statement of the Result

Let $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$, where $\mathscr{H}_1$ and $\mathscr{H}_2$ have respective dimensions k and m, with $k < m < \infty$. For any given density matrix ρ_1 on $\mathscr{H}_1$, consider the set

$$\mathscr{R}(\rho_1) = \left\{\psi \in \mathscr{S}(\mathscr{H}) : \rho_1^{\mathrm{red}}(\psi) = \rho_1\right\}, \tag{29}$$

where $\rho_1^{\mathrm{red}}(\psi) = \mathrm{tr}_2|\psi\rangle\langle\psi|$ is the reduced density matrix for the wave function ψ. There is a natural notion of (normalized) uniform measure u_{ρ_1} on $\mathscr{R}(\rho_1)$; we give its precise definition in Section 5.1.3.

We claim that for fixed k and large m, the distribution μ_1^{ψ} of the conditional wave function Ψ_1 of system 1, defined by (4) and (5) for a basis $\{|q_2\rangle\}$ of $\mathscr{H}_2$, is close to $GAP(\rho_1)$ for the overwhelming majority, relative to u_{ρ_1}, of vectors $\psi \in \mathscr{H}$ with reduced density matrix ρ_1. More precisely:

For every $\varepsilon > 0$ and every bounded continuous function $f : \mathscr{S}(\mathscr{H}_1) \to \mathbb{R}$,

$$u_{\rho_1}\Big\{\psi \in \mathscr{R}(\rho_1) : \left|\mu_1^{\psi}(f) - GAP(\rho_1)(f)\right| < \varepsilon\Big\} \to 1 \quad \textit{as } m \to \infty, \tag{30}$$

regardless of how the basis $\{|q_2\rangle\}$ is chosen.

Here we use the notation

$$\mu(f) := \int\limits_{\mathscr{S}(\mathscr{H})} \mu(d\psi)\, f(\psi). \tag{31}$$

5.1.2 Measure on $\mathscr{H}$ Versus Density Matrix

It is important to resist the temptation to translate u_{ρ_1} into a density matrix in $\mathscr{H}$. As mentioned in the introduction, to every probability measure μ on $\mathscr{S}(\mathscr{H})$ there corresponds a density matrix ρ_μ in $\mathscr{H}$, given by (1), which contains all the empirically accessible information about an ensemble with distribution μ. It may therefore seem a natural step to consider, instead of the measure $\mu = u_{\rho_1}$, directly its density matrix $\rho_\mu = \frac{1}{m}\rho_1 \otimes I_2$, where I_2 is the identity on $\mathscr{H}_2$. But since our result concerns properties of most wave functions relative to μ, it cannot be formulated in terms of the density matrix ρ_μ. In particular, the corresponding statement relative to another measure $\mu' \neq \mu$ on $\mathscr{S}(\mathscr{H})$ with the same density matrix $\rho_{\mu'} = \rho_\mu$ could be false. Noting that ρ_μ has a basis of eigenstates that are product vectors, we could, for example, take μ' to be a measure concentrated on these eigenstates. For any such state ψ, μ_1^{ψ} is a delta-measure.

5.1.3 Outline of Proof

The result follows, by (5), Lemma 1, and the continuity of $P_* \circ A$, from the corresponding statement about the Gaussian measure $G(\rho_1)$ on $\mathscr{H}_1$ with covariance ρ_1:

For every $\varepsilon > 0$ and every bounded continuous $f : \mathscr{H}_1 \to \mathbb{R}$,

$$u_{\rho_1}\Big\{\psi \in \mathscr{R}(\rho_1) : \big|\bar{\mu}_1^{\psi}(f) - G(\rho_1)(f)\big| < \varepsilon\Big\} \to 1 \quad \textit{as} \;\; m \to \infty\,, \tag{32}$$

where $\bar{\mu}_1^{\psi}$ is the distribution of $\sqrt{m}\,\langle Q_2|\psi\rangle \in \mathscr{H}_1$ (not normalized) with respect to the uniform distribution of $Q_2 \in \{1, \ldots, m\}$.

We sketch the proof of (32) and give the definition of u_{ρ_1}. According to the Schmidt decomposition, every $\psi \in \mathscr{H}$ can be written in the form

$$\psi = \sum_i c_i\, \chi_i \otimes \phi_i\,, \tag{33}$$

where $\{\chi_i\}$ is an orthonormal basis of $\mathscr{H}_1$, $\{\phi_i\}$ an orthonormal system in $\mathscr{H}_2$, and the c_i are coefficients which can be assumed real and nonnegative. From (33) one reads off the reduced density matrix of system 1,

$$\rho_1^{\mathrm{red}} = \sum_i c_i^2\, |\chi_i\rangle\langle\chi_i|\,. \tag{34}$$

As the reduced density matrix is given, $\rho_1^{\mathrm{red}} = \rho_1$, the orthonormal basis $\{\chi_i\}$ and the coefficients c_i are determined (when ρ_1 is nondegenerate) as the eigenvectors and the square-roots of the eigenvalues of ρ_1, and, $\mathscr{R}(\rho_1)$ is in a natural one-to-one correspondence with the set $ONS(\mathscr{H}_2, k)$ of all orthonormal systems $\{\phi_i\}$ in $\mathscr{H}_2$ of cardinality k. (If some of the eigenvalues of ρ_1 vanish, the one-to-one correspondence is with $ONS(\mathscr{H}_2, k')$ where $k' = \dim \mathrm{support}(\rho_1)$.) The Haar measure on the unitary group of $\mathscr{H}_2$ defines the uniform distribution on the set of orthonormal bases of $\mathscr{H}_2$, of which the uniform distribution on $ONS(\mathscr{H}_2, k)$ is a marginal, and thus defines the uniform distribution u_{ρ_1} on $\mathscr{R}(\rho_1)$. (When ρ_1 is degenerate, u_{ρ_1} does not depend upon how the eigenvectors χ_i of ρ_1 are chosen.)

The key idea for establishing (32) from the Schmidt decomposition (33) is this: $\bar{\mu}_1^{\psi}$ is the average of m delta measures with equal weights, $\bar{\mu}_1^{\psi} = m^{-1} \sum_{q_2} \delta_{\psi_1(q_2)}$, located at the points

$$\psi_1(q_2) = \sum_{i=1}^{k} c_i\, \sqrt{m}\, \langle q_2|\phi_i\rangle\, \chi_i\,. \tag{35}$$

Now regard ψ as random with distribution u_{ρ_1}; then the $\psi_1(q_2)$ are m random vectors, and $\bar{\mu}_1^{\psi}$ is their empirical distribution. If the mk coefficients $\langle q_2|\phi_i\rangle$ were *independent*

Gaussian (complex) random variables with (mean zero and) variance m^{-1}, then the $\psi_1(q_2)$ would be m independent drawings of a $G(\rho_1)$-distributed random vector; by the weak law of large numbers, their empirical distribution would usually be close to $G(\rho_1)$; in fact, the probability that $\left|\bar{\mu}_1^{\psi}(f) - G(\rho_1)(f)\right| < \varepsilon$ would converge to 1, as $m \to \infty$.

However, when $\{\phi_i\}$ is a random orthonormal system with uniform distribution as described above, the expansion coefficients $\langle q_2|\phi_i\rangle$ in the decomposition of the ϕ_i's

$$\phi_i = \sum_{q_2} \langle q_2|\phi_i\rangle |q_2\rangle \tag{36}$$

will not be independent—since the ϕ_i's must be orthogonal and since $\|\phi_i\| = 1$. Nonetheless, replacing the coefficients $\langle q_2|\phi_i\rangle$ in (36) by independent Gaussian coefficients $a_i(q_2)$ as described above, we obtain a system of vectors

$$\phi_i' = \sum_{q_2} a_i(q_2)|q_2\rangle \tag{37}$$

that, in the limit $m \to \infty$, form a uniformly distributed orthonormal system: $\|\phi_i'\| \to 1$ (by the law of large numbers) and $\langle \phi_i'|\phi_j'\rangle \to 0$ for $i \neq j$ (since a pair of randomly chosen vectors in a high-dimensional Hilbert space will typically be almost orthogonal). This completes the proof.

5.1.4 Reformulation

While this result *suggests* that $GAP(\rho_\beta)$ is the distribution of the conditional wave function of a system coupled to a heat bath when the wave function of the composite is a typical *fixed* microcanonical wave function, belonging to $\mathscr{H}_{E,\delta}$, it does not quite *imply* it. The reason for this is that $\mathscr{H}_{E,\delta}$ has measure 0 with respect to the uniform distribution on $\mathscr{H}$, even when the latter is finite-dimensional. Nonetheless, there is a simple corollary, or reformulation, of the result that will allow us to cope with microcanonical wave functions.

We have indicated that for our result the choice of basis $\{|q_2\rangle\}$ of $\mathscr{H}_2$ does not matter. In fact, while μ_1^{ψ}, the distribution of the conditional wave function Ψ_1 of system 1, depends upon both $\psi \in \mathscr{H}$ and the choice of basis $\{|q_2\rangle\}$ of $\mathscr{H}_2$, the distribution of μ_1^{ψ} itself, when ψ is u_{ρ_1}-distributed, does not depend upon the choice of basis. This follows from the fact that for any unitary U on $\mathscr{H}_2$

$$\langle U^{-1}q_2|\psi\rangle = \langle q_2|I_1 \otimes U\psi\rangle \tag{38}$$

(and the invariance of the Haar measure of the unitary group of $\mathscr{H}_2$ under left multiplication). It similarly follows from (38) that for fixed $\psi \in \mathscr{H}$, the distribution of μ_1^{ψ}

arising from the uniform distribution ν of the basis $\{|q_2\rangle\}$, in the set $ONB(\mathscr{H}_2)$ of all orthonormal bases of $\mathscr{H}_2$, is the same as the distribution of μ_1^ψ arising from the uniform distribution u_{ρ_1} of ψ with a fixed basis (and the fact that the Haar measure is invariant under $U \mapsto U^{-1}$). We thus have the following corollary:

Let $\psi \in \mathscr{H}$ and let $\rho_1 = \mathrm{tr}_2|\psi\rangle\langle\psi|$ be the corresponding reduced density matrix for system 1. Then for a typical basis $\{|q_2\rangle\}$ of $\mathscr{H}_2$, the conditional wave function Ψ_1 of system 1 is approximately $GAP(\rho_1)$-distributed when m is large: For every $\varepsilon > 0$ and every bounded continuous function $f : \mathscr{S}(\mathscr{H}_1) \to \mathbb{R}$,

$$\nu\Big\{\{|q_2\rangle\} \in ONB(\mathscr{H}_2) : \big|\mu_1^\psi(f) - GAP(\rho_1)(f)\big| < \varepsilon\Big\} \to 1 \quad as \;\; \dim(\mathscr{H}_2) \to \infty\,. \quad (39)$$

5.2 Typicality of $GAP(\rho_\beta)$ for a Subsystem of a Large System in the Microcanonical Ensemble

It is an immediate consequence of the result of Section 5.1.4 that for any fixed microcanonical wave function ψ for a system coupled to a (large) heat bath, the conditional wave function Ψ_1 of the system will be approximately GAP-distributed. When this is combined with the “canonical typicality” described near the beginning of Section 5, we obtain the following result:

Consider a system with finite-dimensional Hilbert space $\mathscr{H}_1$ coupled to a heat bath with finite-dimensional Hilbert space $\mathscr{H}_2$. Suppose that the coupling is weak, so that we can write $H = H_1 \otimes I_2 + I_1 \otimes H_2$ on $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$, and that the heat bath is large, so that the eigenvalues of H_2 are close. Then for any wave function ψ that is typical relative to the microcanonical measure $u_{E,\delta}$, the distribution μ_1^ψ of the conditional wave function Ψ_1, defined by (4) and (5) for a typical basis $\{|q_2\rangle\}$ of the heat bath, is close to $GAP(\rho_\beta)$ for suitable $\beta = \beta(E)$, where $\rho_\beta = \rho_{\mathscr{H}_1,H_1,\beta}$. In other words, in the thermodynamic limit, in which the volume V of the heat bath and $dim(\mathscr{H}_2)$ go to infinity and $E/V = e$ is constant, we have that for all $\varepsilon, \delta > 0$, and for all bounded continuous functions $f : \mathscr{S}(\mathscr{H}_1) \to \mathbb{R}$,

$$u_{E,\delta} \times \nu\Big\{(\psi, \{|q_2\rangle\}) \in \mathscr{S}(\mathscr{H}) \times ONB(\mathscr{H}_2) : \big|\mu_1^\psi(f) - GAP(\rho_\beta)(f)\big| < \varepsilon\Big\} \to 1 \quad (40)$$

where $\beta = \beta(e)$.

We note that if $\{|q_2\rangle\}$ were an energy eigenbasis rather than a typical basis, the result would be false.

6 Remarks

6.1 Other Candidates for the Canonical Distribution

We review in this section other distributions that have been, or may be, considered as possible candidates for the distribution of the wave function of a system from a canonical ensemble.

6.1.1 A Distribution on the Eigenvectors

One possibility, which goes back to von Neumann [25, p. 329], is to consider $\mu(d\psi)$ as concentrated on the eigenvectors of ρ; we denote this distribution $EIG(\rho)$ after the first letters of "eigenvector"; it is defined as follows. Suppose first that ρ is nondegenerate. To select an $EIG(\rho)$-distributed vector, pick a unit eigenvector $|n\rangle$, so that $\rho|n\rangle = p_n|n\rangle$, with probability p_n and randomize its phase. This definition can be extended in a natural way to degenerate ρ:

$$EIG(\rho) = \sum_{p \in \mathrm{spec}(\rho)} p \dim \mathscr{H}_p \; u_{\mathscr{S}(\mathscr{H}_p)}, \tag{41}$$

where $\mathscr{H}_p$ denotes the eigenspace of ρ associated with eigenvalue p. The measure $EIG(\rho)$ is concentrated on the set $\bigcup_p \mathscr{H}_p$ of eigenvectors of ρ, which for the canonical $\rho = \rho_{\mathscr{H},H,\beta}$ coincides with the set of eigenvectors of H; it is a mixture of the microcanonical distributions $u_{\mathscr{S}(\mathscr{H}_p)}$ on the eigenspaces of H in the same way as in classical mechanics the canonical distribution on phase space is a mixture of the microcanonical distributions.

Note that $EIG(\rho_{E,\delta}) = u_{E,\delta}$, and that in particular $EIG(\rho_{E,\delta})$ is not, when H is nondegenerate, the uniform distribution $\mu_{E,\delta}$ on the energy eigenstates with energies in $[E, E+\delta]$, against which we have argued in the introduction.

The distribution $EIG(\rho)$ has the same properties as those of $GAP(\rho)$ described in Properties 1–3, except when ρ is degenerate:

The measures $EIG(\rho)$ are such that (a) they have the right density matrix: $\rho_{EIG(\rho)} = \rho$; (b) they are covariant: $U_* EIG(\rho) = EIG(U\rho U^*)$; (c) they are hereditary at nondegenerate ρ: when $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$ and ρ is nondegenerate and uncorrelated, $\rho = \rho_1 \otimes \rho_2$, then $EIG(\rho)$ has marginal (i.e., distribution of the conditional wave function) $EIG(\rho_1)$.

Proof. (a) and (b) are obvious. For (c) let, for $i = 1, 2$, $|n_i\rangle$ be a basis consisting of eigenvectors of ρ_i with eigenvalues $p^{(i)}_{n_i}$. Note that the tensor products $|n_1\rangle \otimes |n_2\rangle$ are eigenvectors of ρ with eigenvalues $p^{(1)}_{n_1} p^{(2)}_{n_2}$, and by nondegeneracy all eigenvectors of ρ are of this form up to a phase factor. Since an $EIG(\rho)$-distributed random vector Ψ is almost surely an eigenvector of ρ, we have $\Psi = e^{i\Theta}|N_1\rangle|N_2\rangle$ with random N_1, N_2, and Θ. The conditional wave function Ψ_1 is, up to the phase, the eigenvector $|N_1\rangle$ of ρ_1 occurring as the first factor in Ψ. The probability of obtaining $N_1 = n_1$ is $\sum_{n_2} p^{(1)}_{n_1} p^{(2)}_{n_2} = p^{(1)}_{n_1}$.[6] $\Box$

In contrast, for a *degenerate* $\rho = \rho_1 \otimes \rho_2$ the conditional wave function need not be $EIG(\rho_1)$-distributed, as the following example shows. Suppose ρ_1 and ρ_2 are non-degenerate but $p^{(1)}_{n_1} p^{(2)}_{n_2} = p^{(1)}_{m_1} p^{(2)}_{m_2}$ for some $n_1 \neq m_1$; then an $EIG(\rho)$-distributed Ψ, whenever it happens to be an eigenvector associated with eigenvalue $p^{(1)}_{n_1} p^{(2)}_{n_2}$, is of the form $c|n_1\rangle|n_2\rangle + c'|m_1\rangle|m_2\rangle$, almost surely with nonvanishing coefficients c and c'; as a consequence, the conditional wave function is a multiple of $c|n_1\rangle\langle Q_2|n_2\rangle + c'|m_1\rangle\langle Q_2|m_2\rangle$, which is, for typical Q_2 and unless $|n_2\rangle$ and $|m_2\rangle$ have disjoint supports, a nontrivial superposition of eigenvectors $|n_1\rangle$, $|m_1\rangle$ with different eigenvalues—and thus cannot arise from the $EIG(\rho_1)$ distribution.[7]

Note also that $EIG(\rho)$ is discontinuous as a function of ρ at every degenerate ρ; in other words, $EIG(\rho_{\mathscr{H},H,\beta})$ is, like $\mu_{E,\delta}$, unstable against small perturbations of the Hamiltonian. (And, as with $\mu_{E,\delta}$, this fact, quite independently of the considerations on behalf of GAP-measures in Sections 4 and 5, suggests against using $EIG(\rho_\beta)$ as a thermal equilibrium distribution.) Moreover, $EIG(\rho)$ is highly concentrated, generically on a one-dimensional subset of $\mathscr{S}(\mathscr{H})$, and in the case of a finite-dimensional Hilbert space $\mathscr{H}$ fails to be absolutely continuous relative to the uniform distribution $u_{\mathscr{S}(\mathscr{H})}$ on the unit sphere.

For further discussion of families $\mu(\rho)$ of measures satisfying the analogues of Properties 1–3, see Section 6.2.

6.1.2 An Extremal Distribution

Here is another distribution on $\mathscr{H}$ associated with the density matrix ρ. Let the random vector Ψ be

$$\Psi = \sum_{p \in \mathrm{spec}(\rho)} \sqrt{p}\, \Psi_p, \tag{42}$$

the Ψ_p being independent random vectors with distributions $u_{\mathscr{S}(\mathscr{H}_p)}$. In case all eigenvalues are nondegenerate, this means the coefficients Z_n of Ψ, $\Psi = \sum_n Z_n |n\rangle$, have independent uniform phases but fixed moduli $|Z_n| = \sqrt{p_n}$—in sharp contrast with the moduli when Ψ is $GAP(\rho)$-distributed. And in contrast to the measure $EIG(\rho)$ considered in the previous subsection, the weights p_n in the density matrix now come from the fixed size of the coefficients of Ψ when it is decomposed into the eigenvectors of ρ, rather

[6] The relevant condition for (c) follows from nondegeneracy but is weaker: it is that the eigenvalues of ρ_1 and ρ_2 are multiplicatively independent, in the sense that $p^{(1)}_{n_1} p^{(2)}_{n_2} = p^{(1)}_{m_1} p^{(2)}_{m_2}$ can occur only trivially, i.e., when $p^{(1)}_{n_1} = p^{(1)}_{m_1}$ and $p^{(2)}_{n_2} = p^{(2)}_{m_2}$. In particular, the nondegeneracy of ρ_1 and ρ_2 is irrelevant.

[7] A property weaker than (c) does hold for $EIG(\rho)$ also in the case of the degeneracy of $\rho = \rho_1 \otimes \rho_2$: if the orthonormal basis $\{|q_2\rangle\}$ used in the definition of conditional wave function consists of eigenvectors of ρ_2, then the distribution of the conditional wave function is $EIG(\rho_1)$.

than from the probability with which these eigenvectors are chosen. This measure, too, is stationary under any unitary evolution that leaves ρ invariant. In particular, it is stationary in the thermal case $\rho = \rho_{\mathscr{H},H,\beta}$, and for generic H it is an extremal stationary measure as characterized in Section 3.2.1; in fact it is, in the notation of the last paragraph of Section 3.2.1, λ_p with $p(E_n) = (1/Z)\exp(-\beta E_n)$.

This measure, too, is highly concentrated: For a Hilbert space $\mathscr{H}$ of finite dimension k, it is supported by a submanifold of real dimension $2k - m$ where m is the number of distinct eigenvalues of H, hence generically it is supported by a submanifold of just half the dimension of $\mathscr{H}$.

6.1.3 The Distribution of Guerra and Loffredo

In [10], Guerra and Loffredo consider the canonical density matrix ρ_β for the one-dimensional harmonic oscillator and want to associate with it a diffusion process on the real line, using stochastic mechanics [18, 9]. Since stochastic mechanics associates a process with every wave function, they achieve this by finding a measure μ_β on $\mathscr{S}(L^2(\mathbb{R}))$ whose density matrix is ρ_β.

They propose the following measure μ_β, supported by coherent states. With every point (q,p) in the classical phase space $\mathbb{R}^2$ of the harmonic oscillator there is associated a coherent state

$$\psi_{q,p}(x) = (2\pi\sigma^2)^{-1/4}\,\exp\Big(-\frac{(x-q)^2}{4\sigma^2} + \frac{i}{\hbar}xp - \frac{i}{2\hbar}pq\Big) \tag{43}$$

with $\sigma^2 = \hbar/2m\omega$, thus defining a mapping $C : \mathbb{R}^2 \to \mathscr{S}(L^2(\mathbb{R}))$, $C(q,p) = \psi_{q,p}$. Let $H(q,p) = p^2/2m + \frac{1}{2}m\omega^2 q^2$ be the classical Hamiltonian function, and consider the classical canonical distribution at inverse temperature β',

$$\rho^{\text{class}}_{\beta'}(dq \times dp) = \frac{1}{Z'}e^{-\beta' H(q,p)}\,dq\,dp\,, \quad Z' = \int_{\mathbb{R}^2} dq\,dp\,e^{-\beta' H(q,p)}\,. \tag{44}$$

Let $\beta' = \frac{e^{\beta\hbar\omega}-1}{\hbar\omega}$. Then $\mu_\beta = C_* \rho^{\text{class}}_{\beta'}$ is the distribution on coherent states arising from $\rho^{\text{class}}_{\beta'}$. The density matrix of μ_β is ρ_β [10].

This measure is concentrated on a 2-dimensional submanifold of $\mathscr{S}(L^2(\mathbb{R}))$, namely on the set of coherent states (the image of C). Note also that not every density matrix ρ on $L^2(\mathbb{R})$ can arise as the density matrix of a distribution on the set of coherent states; for example, a pure state $\rho = |\psi\rangle\langle\psi|$ can arise in this way if and only if ψ is a coherent state.

6.1.4 The Distribution Maximizing an Entropy Functional

In a similar spirit, one may consider, on a finite-dimensional Hilbert space $\mathscr{H}$, the distribution $\gamma(d\psi) = f(\psi)\, u_{\mathscr{S}(\mathscr{H})}(d\psi)$ that maximizes the Gibbs entropy functional

$$\mathscr{G}[f] = -\int\limits_{\mathscr{S}(\mathscr{H})} u(d\psi)\;\; f(\psi)\, \log f(\psi) \tag{45}$$

under the constraints that γ be a probability distribution with mean 0 and covariance $\rho_{\mathscr{H},H,\beta}$:

$$f \geq 0 \tag{46a}$$

$$\int\limits_{\mathscr{S}(\mathscr{H})} u(d\psi)\, f(\psi) = 1 \tag{46b}$$

$$\int\limits_{\mathscr{S}(\mathscr{H})} u(d\psi)\, f(\psi)\, |\psi\rangle = 0 \tag{46c}$$

$$\int\limits_{\mathscr{S}(\mathscr{H})} u(d\psi)\, f(\psi)\, |\psi\rangle\langle\psi| = \rho_{\mathscr{H},H,\beta}\,. \tag{46d}$$

A standard calculation using Lagrange multipliers leads to

$$f(\psi) = \exp\langle\psi|L|\psi\rangle \tag{47}$$

with L a self-adjoint matrix determined by (46b) and (46d); comparison with (18b) shows that γ is not a GAP measure. (We remark, however, that another Gibbs entropy functional, $\mathscr{G}'[f] = -\int_{\mathscr{H}} \lambda(d\psi)\;f(\psi)\,\log f(\psi)$, based on the Lebesgue measure λ on $\mathscr{H}$ instead of $u_{\mathscr{S}(\mathscr{H})}$, is maximized, under the constraints that the mean be 0 and the covariance be ρ, by the Gaussian measure, $f(\psi)\,\lambda(d\psi) = G(\rho)(d\psi)$.) There is no apparent reason why the family of γ measures should be hereditary.

The situation is different for the microcanonical ensemble: here, the distribution $u_{E,\delta} = GAP(\rho_{E,\delta})$ that we propose is in fact the maximizer of the appropriate Gibbs entropy functional $\mathscr{G}''$. Which functional is that? Since any measure $\gamma(d\psi)$ on $\mathscr{S}(\mathscr{H})$ whose covariance matrix is the projection $\rho_{E,\delta} = \text{const.}\, 1_{[E,E+\delta]}(H)$ must be concentrated on the subspace $\mathscr{H}_{E,\delta}$ and thus cannot be absolutely continuous (possess a density) relative to $u_{\mathscr{S}(\mathscr{H})}$, we consider instead its density relative to $u_{\mathscr{S}(\mathscr{H}_{E,\delta})} = u_{E,\delta}$, that is, we consider $\gamma(d\psi) = f(\psi)\, u_{E,\delta}(d\psi)$ and set

$$\mathscr{G}''[f] = -\int\limits_{\mathscr{S}(\mathscr{H}_{E,\delta})} u_{E,\delta}(d\psi)\, f(\psi)\, \log f(\psi)\,. \tag{48}$$

Under the constraints that the probability measure γ have mean 0 and covariance $\rho_{E,\delta}$, $\mathscr{G}''[f]$ is maximized by $f \equiv 1$, or $\gamma = u_{E,\delta}$; in fact even without the constraints on γ, $\mathscr{G}''[f]$ is maximized by $f \equiv 1$.

6.1.5 The Distribution of Brody and Hughston

Brody and Hughston [5] have proposed the following distribution μ to describe thermal equilibrium. They observe that the projective space arising from a finite-dimensional Hilbert space, endowed with the dynamics arising from the unitary dynamics on Hilbert space, can be regarded as a classical Hamiltonian system with Hamiltonian function $H(\mathbb{C}\psi) = \langle\psi|H|\psi\rangle/\langle\psi|\psi\rangle$ (and symplectic form arising from the Hilbert space structure). They then define μ to be the classical canonical distribution of this Hamiltonian system, i.e., to have density proportional to $\exp(-\beta H(\mathbb{C}\psi))$ relative to the uniform volume measure on the projective space (which can be obtained from the symplectic form or, alternatively, from $u_{\mathscr{S}(\mathscr{H})}$ by projection from the sphere to the projective space). However, this distribution leads to a density matrix, different from the usual one ρ_β given by (3), that does not describe the canonical ensemble.

6.2 A Uniqueness Result for $GAP(\rho)$

As $EIG(\rho)$ is a family of measures satisfying Properties 1–3 for *most* density matrices ρ, the question arises whether there is any family of measures, besides $GAP(\rho)$, satisfying these properties for *all* density matrices. We expect that the answer is no, and formulate the following uniqueness conjecture: *Given, for every Hilbert space $\mathscr{H}$ and every density matrix ρ on $\mathscr{H}$, a probability measure $\mu(\rho)$ on $\mathscr{S}(\mathscr{H})$ such that Properties 1–3 remain true when $GAP(\rho)$ is replaced by $\mu(\rho)$, then $\mu(\rho) = GAP(\rho)$.* In other words, we conjecture that $\mu = GAP(\rho)$ is the only hereditary covariant inverse of (1).

This is in fact true when we assume in addition that the mapping $\mu : \rho \mapsto \mu(\rho)$ is suitably continuous. Here is the argument: When ρ is a multiple of a projection, $\rho = (\dim \mathscr{H}')^{-1} P_{\mathscr{H}'}$ for a subspace $\mathscr{H}' \subseteq \mathscr{H}$, then $\mu(\rho)$ must be, by covariance $U_*\mu(\rho) = \mu(U\rho U^*)$, the uniform distribution on $\mathscr{S}(\mathscr{H}')$, and thus $\mu(\rho) = GAP(\rho)$ in this case. Consider now a composite of a system (system 1) and a large heat bath (system 2) with Hilbert space $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$ and Hamiltonian $H = H_1 \otimes I_2 + I_1 \otimes H_2$, and consider the microcanonical density matrix $\rho_{E,\delta}$ for this system. By equivalence of ensembles, we have for suitable $\beta > 0$ that $\rho_{E,\delta} \approx \rho_{\mathscr{H},H,\beta} = \rho_\beta^{(1)} \otimes \rho_\beta^{(2)}$ where $\rho_\beta^{(i)} = \rho_{\mathscr{H}_i,H_i,\beta}$. By the continuity of μ and GAP,

$$\mu\big(\rho_\beta^{(1)} \otimes \rho_\beta^{(2)}\big) \approx \mu(\rho_{E,\delta}) = GAP(\rho_{E,\delta}) \approx GAP(\rho_\beta^{(1)} \otimes \rho_\beta^{(2)})\,.$$

Now consider, for a wave function Ψ with distribution $\mu\big(\rho_\beta^{(1)}\otimes\rho_\beta^{(2)}\big)$ respectively $GAP(\rho_\beta^{(1)}\otimes\rho_\beta^{(2)})$, the distribution of the conditional wave function Ψ_1: by heredity, this is $\mu(\rho_\beta^{(1)})$ respectively $GAP(\rho_\beta^{(1)})$. Since the distribution of Ψ_1 is a continuous function of the distribution of Ψ, we thus have that $\mu(\rho_\beta^{(1)}) \approx GAP(\rho_\beta^{(1)})$. Since we can make the degree of approximation arbitrarily good by making the heat bath sufficiently large, we must have that $\mu(\rho_\beta^{(1)}) = GAP(\rho_\beta^{(1)})$. For any density matrix ρ on $\mathscr{H}_1$ that does not have zero among its eigenvalues, there is an H_1 such that $\rho = \rho_\beta^{(1)} = Z^{-1}\exp(-\beta H_1)$ for $\beta = 1$, and thus we have that $\mu(\rho) = GAP(\rho)$ for such a ρ; since these are dense, we have that $\mu(\rho) = GAP(\rho)$ for all density matrices ρ on $\mathscr{H}_1$. Since $\mathscr{H}_1$ is arbitrary we are done.

6.3 Dynamics of the Conditional Wave Function

Markov processes in Hilbert space have long been considered (see [4] for an overview), particularly diffusion processes and piecewise deterministic (jump) processes. This is often done for the purpose of numerical simulation of a master equation for the density matrix, or as a model of continuous measurement or of spontaneous wave function collapse. Such processes could arise as follows.

Since the conditional wave function Ψ_1 arises from the wave function $\langle q_2|\psi\rangle$ by inserting a random coordinate Q_2 for the second variable (and normalizing), any dynamics (i.e., time evolution) for Q_2, described by a curve $t \mapsto Q_2(t)$ and preserving the quantum probability distribution of Q_2, for example, as given by Bohmian mechanics [6], gives rise to a dynamics for the conditional wave function, $t \mapsto \Psi_1(t) = \mathcal{N}(t)\,\langle Q_2(t)|\psi(t)\rangle$, where $\psi(t)$ evolves according to Schrödinger's equation and $\mathcal{N}(t) = \|\langle Q_2(t)|\psi(t)\rangle\|^{-1}$ is the normalizing factor. In this way one obtains a stochastic process (a random path) in $\mathscr{S}(\mathscr{H}_1)$. In the case considered in Section 4, in which $\mathscr{H}_2$ corresponds to a large heat bath, this process must have $GAP(\rho_{\mathscr{H}_1,H_1,\beta})$ as an invariant measure. It would be interesting to know whether this process is approximately a simple process in $\mathscr{S}(\mathscr{H}_1)$, perhaps a diffusion process, perhaps one of the Markov processes on Hilbert space considered already in the literature.

7 The Two-Level System as a Simple Example

In this last section, we consider a two-level system, with $\mathscr{H} = \mathbb{C}^2$ and

$$H = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|, \tag{49}$$

and calculate the joint distribution of the energy coefficients $Z_1 = \langle 1|\Psi\rangle$ and $Z_2 = \langle 2|\Psi\rangle$ for a $GAP(\rho_\beta)$-distributed Ψ as explicitly as possible. We begin with a general finite-dimensional system, $\mathscr{H} = \mathbb{C}^k$, and specialize to $k = 2$ later.

One way of describing the distribution of Ψ is to give its density relative to the hypersurface area measure u on $\mathscr{S}(\mathbb{C}^k)$; this we did in (18). Another way of describing the joint distribution of the Z_n is to describe the joint distribution of their moduli $|Z_n|$, or of $|Z_n|^2$, as the phases of the Z_n are independent (of each other and of the moduli) and uniformly distributed, see (22).

Before we determine the distribution of $|Z_n|^2$, we repeat that its expectation can be computed easily. In fact, for any $\phi \in \mathscr{H}$ we have

$$\mathbb{E}\big|\langle\phi|\Psi\rangle\big|^2 = \int\limits_{\mathscr{S}(\mathscr{H})} GAP(\rho_\beta)(d\psi)\,\big|\langle\phi|\psi\rangle\big|^2 \overset{(1)}{=} \langle\phi|\rho_\beta|\phi\rangle \overset{(3)}{=} \frac{1}{Z(\beta)}\langle\phi|e^{-\beta H}|\phi\rangle.$$

Thus, for $|\phi\rangle = |n\rangle$, we obtain $\mathbb{E}|Z_n|^2 = e^{-\beta E_n}/\mathrm{tr}\, e^{-\beta H}$.

For greater clarity, from now on we write Z_n^{GAP} instead of Z_n. A relation similar to that between $GAP(\rho)$, $GA(\rho)$, and $G(\rho)$ holds between the joint distributions of the $|Z_n^{GAP}|^2$, of the $|Z_n^{GA}|^2$, and of the $|Z_n^{G}|^2$. The joint distribution of the $|Z_n^G|^2$ is very simple: they are independent and exponentially distributed with means $p_n = e^{-\beta E_n}/Z(\beta)$. Since the density of GA relative to G, $dGA/dG = \sum_n |z_n|^2$, is a function of the moduli alone, and since, according to (22), $GA = GA_{\mathrm{phases}} \times GA_{\mathrm{moduli}}$, we have that

$$GA_{\mathrm{moduli}} = \sum_n |z_n|^2\, G_{\mathrm{moduli}}.$$

Thus,

$$\mathbb{P}\big(|Z_1^{GA}|^2 \in ds_1, \dots, |Z_k^{GA}|^2 \in ds_k\big) = \frac{s_1 + \dots + s_k}{p_1 \cdots p_k} \exp\Big(-\sum_{n=1}^{k} \frac{s_n}{p_n}\Big) ds_1 \cdots ds_k, \tag{50}$$

where each $s_n \in (0,\infty)$. Finally, the $|Z_n^{GAP}|^2$ arise by normalization,

$$|Z_n^{GAP}|^2 = \frac{|Z_n^{GA}|^2}{\sum\limits_{n'} |Z_{n'}^{GA}|^2}. \tag{51}$$

We now specialize to the two-level system, $k = 2$. Since $|Z_1^{GAP}|^2 + |Z_2^{GAP}|^2 = 1$, it suffices to determine the distribution of $|Z_1^{GAP}|^2$, for which we give an explicit formula in (52c) below. We want to obtain the marginal distribution of (51) from the joint distribution of the $|Z_n^{GA}|^2$ in $(0,\infty)^2$, the first quadrant of the plane, as given by (50). To this end, we introduce new coordinates in the first quadrant:

$$s = \frac{s_1}{s_1 + s_2}, \quad \lambda = s_1 + s_2,$$

where $\lambda > 0$ and $0 < s < 1$. Conversely, we have $s_1 = s\lambda$ and $s_2 = (1-s)\lambda$, and the area element transforms according to

$$ds_1\, ds_2 = \Big|\det \frac{\partial(s_1, s_2)}{\partial(s,\lambda)}\Big| ds\, d\lambda = \lambda\, ds\, d\lambda.$$

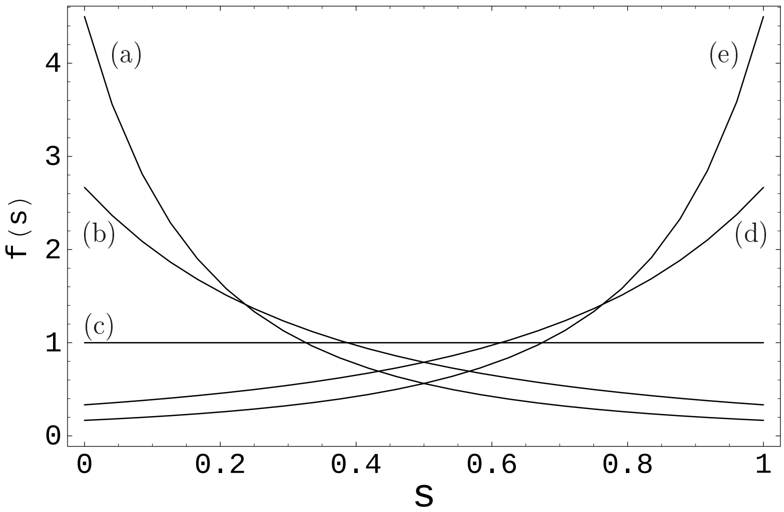

Figure 1: Plot of the distribution density function $f(s)$ of $|Z_1|^2$, defined in (52c), for various values of the parameter $\delta = \exp(\beta(E_2 - E_1))$: (a) $\delta = 1/3$, (b) $\delta = 1/2$, (c) $\delta = 1$, (d) $\delta = 2$, (e) $\delta = 3$.

Therefore, using

$$\int_0^\infty d\lambda\, \lambda^2 e^{-x\lambda} = 2x^{-3} \text{ for } x > 0,$$

we obtain

$$\mathbb{P}\Big(|Z_1^{GAP}|^2 \in ds\Big) = ds \int_0^\infty d\lambda\, \frac{e^{\beta \operatorname{tr} H}}{Z(\beta)} \lambda^2 \exp\Big(-\lambda\big(e^{\beta E_1} s + e^{\beta E_2}(1-s)\big)\Big) = \tag{52a}$$

$$= \frac{2e^{\beta \operatorname{tr} H}}{Z(\beta)} \big(e^{\beta E_1} s + e^{\beta E_2}(1-s)\big)^{-3} ds = \tag{52b}$$

$$= \big(\alpha_1 s + \alpha_2(1-s)\big)^{-3} ds =: f(s)\, ds\,, \quad 0 < s < 1, \tag{52c}$$

with $\alpha_1 = (\delta^{-1}(\delta^{-1}+1)/2)^{1/3}$ and $\alpha_2 = (\delta(\delta+1)/2)^{1/3}$ for $\delta = \exp(\beta(E_2 - E_1))$. The density f of the distribution (52c) of $|Z_1^{GAP}|^2$ is depicted in Figure 1 for various values of δ. For $\delta = 1$, f is identically 1. For $\delta > 1$, we have $\alpha_2 = \delta\alpha_1 > \alpha_1$, so that $\alpha_1 s + \alpha_2(1-s)$ is decreasing monotonically from α_2 at $s = 0$ to α_1 at $s = 1$; hence, f is increasing monotonically from α_2^{-3} to α_1^{-3}. For $\delta < 1$, we have $\alpha_2 < \alpha_1$, and hence f is decreasing monotonically from α_2^{-3} to α_1^{-3}. In all cases f is convex since $f'' \geq 0$.

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