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Geometric Quantum Thermodynamics

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Building on parallels between geometric quantum mechanics and classical mechanics, we explore an alternative basis for quantum thermodynamics that exploits the differential geometry of the underlying state space. We focus on microcanonical and canonical ensembles, looking at the geometric counterpart of Gibbs ensembles for distributions on the space of quantum states. We show that one can define quantum heat and work in an intrinsic way, including single-trajectory work. We reformulate thermodynamic entropy in a way that accords with classical, quantum, and information-theoretic entropies. We give both the First and Second Laws of Thermodynamics and Jarzynki's Fluctuation Theorem. Overall, this results in a more transparent physics than conventionally available. The mathematical structure and physical intuitions underlying classical and quantum dynamics are seen to be closely aligned. The experimental relevance is brought out via a stochastic model for chiral molecules (in the two-state approximation) and Josephson junctions. Numerically, we demonstrate this invariably leads to the emergence of the geometric canonical ensemble.

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I. INTRODUCTION

Geometric quantum mechanics (GQM) exploits the tools of differential geometry to analyze the phenomenology of quantum systems. It does so by focusing on the interplay between statistics and geometry of quantum state space.

For finite-dimensional quantum systems—that we consider here—the state space $\mathcal{H}$ is isomorphic to a complex projective space $\mathbb{C}P^n$ of dimension $n = D - 1$, where $D \coloneqq \dim \mathcal{H}$. Our goal is to explore the statistical and thermodynamic consequences of the geometric approach. In particular, structural and informational properties can be properly formulated. And, the close parallels in the mathematical foundations of classical and quantum dynamics become clear.

To the best of our knowledge, the development of the geometric formalisms started with early insights from Strocchi [1] and then work by Kibble [2], Marsden [3], Heslot [4], Gibbons [5], Ashtekar and Shilling [6, 7], and a host of others [8–18]. Although geometric tools for quantum mechanics are an interesting topic in their own right, the following explores their consequences for statistical mechanics and nonequilibrium thermodynamics.

As one example in this direction, Brody and Hughston [19–21] showed that a statistical mechanics treatment of quantum systems based on the geometric formulation differs from standard quantum statistical mechanics: The former can describe phase transitions away from the thermodynamic limit, the latter not [22]. This arises, most directly, since the geometric formulation puts quantum mechanics on the same footing as the classical mechanics of phase space [1, 4], bringing to light the symplectic geometry of quantum state space. It is then straightforward to build on the principles of classical statistical mechanics to layout a version of quantum statistical mechanics that takes advantage of such state-space features.

That said, these insights do not come for free. The conundrum of a consistent foundation of thermodynamic behavior arises. On the one hand, we have quantum statistical mechanics—a description of macroscopic behavior that, despite limitations, has proven to be remarkably successful. On the other, transitioning from microphysics to macrophysics via quantum mechanics is conceptually different than via classical mechanics. Consistency between these approaches begs for a conceptually unique route from microphysics to macrophysics.

With this broad perspective in mind, unifying the two coexisting statistical mechanics of quantum systems, though challenging, deserves further attention. To address the challenge, the following advocates a geometric development of a practical, macroscopic companion of geometric quantum statistical mechanics—a geometric quantum thermodynamics.

Beyond foundations, geometric quantum thermodynamics is all the more timely due to recent success in driving thermodynamics down to the mesoscopic scale. There statistical fluctuations, quantum fluctuations, and collective behavior not only cannot be neglected, but are essential. Largely, this push is articulated in two research thrusts: *stochastic thermodynamics* [23, 24] and *quantum thermodynamics* [25, 26]. The following draws ideas and tools from both, in effect showing that geometric tools provide a robust and conceptually-incisive crossover between them.

Our development unfolds as follows. First, it recalls the basic elements of geometric quantum mechanics. Sec-

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ond, it shows how this formalism emerges naturally in a thermodynamic context. Third, it describes our version of the statistical treatment of geometric quantum mechanics—what we refer to as geometric quantum statistical mechanics. Fourth, it builds on this to establish two fundamental equations of geometric quantum thermodynamics. The first is a novel version of the first law of quantum thermodynamics, with its definition of quantum heat and quantum work. The second is a quantum version of Jarzynski's inequality—one that does not require a two-time measurement scheme. Fifth, the development proposes an experiment that highlights geometric quantum thermodynamics' practical relevance. Finally, it expands on the geometric approach's increasing relevance to the thermodynamics of quantum information and computing.

II. GEOMETRIC QUANTUM MECHANICS

Geometric quantum mechanics arose from efforts to exploit differential geometry to probe the often-counterintuitive behaviors of quantum systems. This section summarizes the relevant concepts, adapting them to our needs. Detailed expositions are found in the original literature [1, 2, 4–7, 9–18]. Here, we present the main ideas in a constructive way, focusing on the aspects that are of direct relevance to thermodynamic behavior.

Any statistical mechanics requires an appropriate, workable concept of ensemble. To do this, one identifies ensembles with coordinate-invariant measures on the space of quantum states, a treatment first introduced in Ref. [19]. We call these distributions *geometric quantum states* and in Ref. [27] we give a generic procedure to compute them in a quantum thermodynamic setting of a small system interacting with a large environment.

Achieving this, though, requires a series of technical steps. The first identifies the manifold of pure states and defines their observables. The second introduces a suitable metric, scalar product, and coordinate-invariant volume element for the pure-state manifold. From these, the third step derives the evolution operator and equations of motion. Finally, states are described via functionals that map observables to scalar values. This is done so that the associated ensembles are coordinate-invariant measures.

Our quantum system of interest has Hilbert space $\mathcal{H}$ of finite dimension D. The space of pure states is therefore the *complex projective space* $\mathcal{P}(\mathcal{H}) \sim \mathbb{C}P^{D-1}$ [10]. Given an arbitrary basis $\{|e_\alpha\rangle\}_{\alpha=0}^{D-1}$ a generic pure state is parametrized by D complex homogeneous coordinates Z^α, up to normalization and an overall phase:

$$|\psi\rangle = \sum_{\alpha=0}^{D-1} Z^\alpha |e_\alpha\rangle \ ,$$

where $Z \in \mathbb{C}^D$, $Z \sim \lambda Z$, and $\lambda \in \mathbb{C}/\{0\}$. For example, the pure state Z_{qubit} of a single qubit can be given real coordinates: $Z_{\text{qubit}} = (\sqrt{p}, \sqrt{1-p}e^{i\nu})$. An observable $\mathcal{O}$ is a quadratic real function of the state. It associates to each point of the pure-state manifold $\mathcal{P}(\mathcal{H})$ the expectation value $\langle\psi| \mathcal{O} |\psi\rangle$ of the corresponding operator $\mathcal{O}$ on that state:

$$\mathcal{O}(Z) = \sum_{\alpha,\beta} \mathcal{O}_{\alpha,\beta} Z^\alpha \overline{Z}^\beta \tag{1}$$

and $\mathcal{O}_{\beta,\alpha} = \overline{\mathcal{O}}_{\alpha,\beta}$. And so, $\mathcal{O}(Z) \in \mathbb{R}$.

These complex projective spaces are *Kahler spaces*. This means there is a function K, which in our case is $K = \log Z \cdot \overline{Z}$, from which one obtains both a metric g:

$$g_{\alpha\overline{\beta}} = \frac{1}{2} \partial_\alpha \overline{\partial}_\beta \log Z \cdot \overline{Z} \ ,$$

with $\overline{g_{\alpha\overline{\beta}}} = g_{\beta\alpha}$, and a symplectic two-form:

$$\Omega = 2i g_{\alpha\beta} dZ^\alpha \wedge d\overline{Z}^\beta \ ,$$

using shorthand $\overline{\partial}_\alpha := \partial/\partial \overline{Z}^\alpha$. It is not too hard to see that these two structures are parts of the Hermitian form that defines the scalar product $\langle\psi_1|\psi_2\rangle$ in $\mathcal{H}$. Indeed, using the standard notation, one has [5]:

$$\langle\psi_1|\psi_2\rangle = g(Z_1, Z_2) + i\Omega(Z_1, Z_2) \ ,$$

Each geometric term provides an independent volume element.

Agreement between these volumes, together with invariance under unitary transformations, selects a unique coordinate-invariant volume element dV_{FS} [19], based on the Fubini-Study metric on $\mathbb{C}P^{D-1}$:

$$dV_{FS} = \frac{1}{(D-1)!} \left(\frac{\Omega}{2}\right) \wedge \left(\frac{\Omega}{2}\right) \wedge \ldots \wedge \left(\frac{\Omega}{2}\right) \tag{2a}$$

$$= \sqrt{\det g(Z, \overline{Z})} dZ d\overline{Z} \ . \tag{2b}$$

(See also Ref. [10] for a textbook treatment.) Equipped with this unique volume element, the total volume of the pure-state manifold $\mathbb{C}P^{D-1}$ is [5, 10]:

$$\text{Vol}\left(\mathbb{C}P^n\right) = \frac{\pi^{D-1}}{(D-1)!} \ .$$

Since symplectic geometry is the correct environment in which to formulate classical mechanics, one can see how the geometric formalism brings classical and quantum mechanics closer together—a point previously raised by Strocchi [1] and made particularly clear by Heslot [4]. Indeed, as in classical mechanics, the symplectic two-form Ω is an antisymmetric tensor with two indices that provides Poisson brackets, Hamiltonian vector fields, and the respective dynamical evolution.

Given two functions A and B on manifold $\mathcal{P}(\mathcal{H})$ we have:

$$\begin{aligned}\Omega(A,B) &= \partial_\alpha A \overline{\partial}_\beta B \Omega^{\alpha\beta} \\ &= \{A, B\} \ ,\end{aligned}$$

where we used $\Omega = \frac{1}{2}\Omega_{\alpha\beta} dZ^\alpha \wedge d\overline{Z}^\beta$ and $\Omega^{\alpha\beta} = (\Omega^{-1})_{\alpha\beta}$ is the inverse: $\Omega^{\alpha\gamma}\Omega_{\gamma\beta} = \delta^\alpha_\beta$. Using the symplectic two-form one can show that Schrödinger's unitary evolution under operator H is generated by a Killing vector field V_H as follows:

$$V_H^\alpha = \Omega^{\alpha\beta}\partial_\beta h(Z) \tag{3a}$$

$$\frac{dF}{dt} = \{F, h\} \tag{3b}$$

where $h(Z) = \sum_{\alpha\beta} H_{\alpha\beta} Z^\alpha \overline{Z}^\beta$ and $F : \mathcal{P}(\mathcal{H}) \to \mathbb{R}$ is a real but otherwise arbitrary function. Indeed, it can be shown that Schrödinger's equation is nothing other than Hamilton's equations of motion in disguise [4, 10]:

$$\frac{d\left|\psi_t\right\rangle}{dt} = -iH\left|\psi_t\right\rangle \quad \Longleftrightarrow \quad \frac{dF}{dt} = \{F, h\} \ , \tag{4}$$

for all F. Here, we use units in which $\hbar = 1$.

This framework naturally views a quantum system's states as the functional encoding that associates expectation values with observables; as done in the C^*-algebra formulation of quantum mechanics [28]. Thus, states are described via functionals $P[\mathcal{O}]$ from the algebra $\mathcal{A}$ of observables to the reals:

$$P[\mathcal{O}] = \int_{\mathcal{P}(\mathcal{H})} p(Z)\mathcal{O}(Z) dV_{FS} \in \mathbb{R} \ ,$$

for $p(Z) \geq 0$ and all $\mathcal{O} \in \mathcal{A}$. Here, p is the distribution associated to the functional P. It is important to note here that dV_{FS} and $\mathcal{O}(Z)$ are both invariant under coordinate changes. Thus, for $P[\mathcal{O}]$ to be a scalar, $p(Z)$ must be a scalar itself. A pure state $\left|\psi\right\rangle \in \mathcal{H}$ is represented by a Dirac-delta functional concentrated on a single point of $\mathcal{P}(\mathcal{H})$. However, Dirac delta-functions $\delta(\cdot)$ are not invariant under coordinate changes: They transform with the inverse of the Jacobian: $\delta \to \delta / \det J$.

To build an invariant quantity, then, we divide it by the square root $\sqrt{g}$ of the metric's determinant. This transforms in the same way, making their ratio $\tilde{\delta} = \delta/\sqrt{g}$ an invariant quantity. This is a standard rescaling that turns coordinate-dependent measures, such as Cartesian measure, into coordinate-invariant ones. And, this is how the Fubini-Study measure Eq. (2) is defined from the Cartesian product measure. Thus:

$$\begin{aligned}P_{\psi_0}[\mathcal{O}] &= \int_{\mathcal{P}(\mathcal{H})} \tilde{\delta}[Z - Z_0]\mathcal{O}(Z) dV_{FS} \\ &= \mathcal{O}(Z_0) \\ &= \left\langle\psi_0\right| \mathcal{O} \left|\psi_0\right\rangle \ ,\end{aligned} \tag{5}$$

where:

$$\tilde{\delta}[Z - Z_0] = \frac{1}{\sqrt{g}} \prod_\alpha \delta(Z^\alpha - Z_0^\alpha)$$

and:

$$\delta(Z^\alpha - Z_0^\alpha) = \delta(\mathrm{Re}[Z^\alpha] - \mathrm{Re}[Z_0^\alpha])\delta(\mathrm{Im}[Z^\alpha] - \mathrm{Im}[Z_0^\alpha]) \ .$$

This extends by linearity to ensembles $\rho = \sum_{k=1}^M p_k \left|\psi_k\right\rangle\left\langle\psi_k\right|$ as:

$$\begin{aligned}P_\rho[\mathcal{O}] &= \sum_{h=1}^M p_k \int_{\mathcal{P}(\mathcal{H})} \tilde{\delta}[Z - Z_k]\mathcal{O}(Z) dV_{FS} \\ &= \sum_{h=1}^M p_k \mathcal{O}(Z_k) \\ &= \sum_{h=1}^M p_k \left\langle\psi_k\right| \mathcal{O} \left|\psi_k\right\rangle \ .\end{aligned}$$

It is now quite natural to consider generalized ensembles that correspond to functionals with a continuous measure on the pure-state manifold.

Such ensembles have appeared previously in Refs. [9, 19–21] and elsewhere, where aspects of their properties have been investigated extensively. For our purposes, it will be useful to look at such ensembles from the following point of view.

Consider a probability measure on the natural numbers: $\{p_k\}$ such that $p_k \geq 0$ and $\sum_k p_k = 1$. Now let Z_k be a countable collection of points in $\mathcal{P}(\mathcal{H})$, then $\delta_k(dZ)$ is the Dirac measure concentrated on the point Z_k. Then, given $\{p_k\}$ one can define the measure $\mu(dZ)$ on $\mathcal{P}(\mathcal{H})$ as:

$$\mu(dZ) = \sum_{k=1}^\infty p_k \delta_k(dZ) \ , \tag{6}$$

which gives precise meaning to the notion of a geometric quantum state with support on a countably-infinite number of points. Indeed, with the measure in Eq.(6) and arbitrary observable function $\mathcal{O}(Z)$ one has that:

$$\begin{aligned}P_\infty[\mathcal{O}] &= \int_{\mathcal{P}(\mathcal{H})} \mathcal{O}(Z)\mu(dZ) \\ &= \sum_{k=1}^\infty p_k \mathcal{O}(Z_k) \ .\end{aligned}$$

In more general terms, calling $\mathcal{B}$ the Borel σ-algebra of the open sets of $\mathcal{P}(\mathcal{H})$, then, this procedure defines a measure μ on $\mathcal{P}(\mathcal{H})$ such that for a set $S \in \mathcal{B}$ one has:

$$\begin{aligned}\mu(S) &= \int_S \mu(dZ) \\ &= \sum_{k=1}^{\infty} p_k I(Z_k \in S) \ ,\end{aligned}$$

where $I(Z_k \in S)$ is the indicator function which is 1 if $Z_k \in S$ and zero otherwise.

The resulting geometric quantum state has all the properties desired of an appropriately-generalized pure-state ensemble: It preserves normalization and convexity of linear combinations, each of its elements are invariant under coordinate changes, and the entire functional P_∞ is also invariant under unitary transformations. With some abuse of language, we will often refer to both the functional P and their underlying measure μ as geometric quantum states.

III. GEOMETRIC QUANTUM STATE AND THE THERMODYNAMIC LIMIT

We are now equipped to address how the geometric formalism arises quite naturally for subsystems of a larger system in a pure state; in particular, in a quantum thermodynamic setting.

If we have a bipartite system $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ and $\left|\psi_{AB}\right\rangle = \sum_{\alpha,i} \psi^{\alpha i}_{AB} \left|a_\alpha\right\rangle \left|b_i\right\rangle \in \mathcal{H}_{AB}$, the partial trace over the subsystem B is:

$$\rho^A = \sum_{\alpha,\beta=1}^{d_A} \rho^A_{\alpha\beta} \left|a_\alpha\right\rangle\!\left\langle a_\beta\right| \ ,$$

where:

$$\begin{aligned}\rho^A_{\alpha\beta} &= \sum_{i=1}^{d_B} \psi^{\alpha i}\overline{\psi}^{\beta i} \\ &= (\psi\psi^\dagger)_{\alpha\beta} \ .\end{aligned}$$

d_A and d_B are A's and B's dimensions, respectively. Hence, we can write the partial trace as:

$$\rho^A = \sum_{j=1}^{d_B} \left|v_j\right\rangle\!\left\langle v_j\right| \ ,$$

with $\left|v_i\right\rangle \in \mathcal{H}_A$ given as:

$$\left|v_i\right\rangle := \sum_{\alpha=1}^{d_A} \psi^{\alpha i} \left|a_\alpha\right\rangle \ .$$

However, $\left|v_j\right\rangle$ is not normalized. To address this, we notice that:

$$\begin{aligned}\left\langle v_j | v_k\right\rangle &= (\psi^\dagger\psi)_{jk} \\ &= \rho^B_{jk} \\ &= \left\langle b_j\right| \rho^B \left|b_k\right\rangle \ .\end{aligned}$$

This gives:

$$\begin{aligned}p^B_k &= \rho^B_{kk} \\ &= \sum_{\alpha=1}^{d_A} \left|\psi^{\alpha k}\right|^2 \ .\end{aligned}$$

We see that $\left\langle v_j | v_k\right\rangle$ is a Gramian matrix of vectors $\left|v_j\right\rangle \in \mathcal{H}_A$ that conveys the information about the reduced state ρ^B on the subspace $\mathcal{H}_A$. Though the vectors $\left|v_k\right\rangle$ are not normalized, we readily define their normalized counterpart:

$$\begin{aligned}\left|\chi_k\right\rangle &:= \frac{\left|v_k\right\rangle}{\sqrt{\left\langle v_k | v_k\right\rangle}} \\ &= \sum_{\alpha=1}^{d_A} \frac{\psi^{\alpha k}}{\sqrt{\sum_{\beta=1}^{d_A} \left|\psi^{\beta k}\right|^2}} \left|a_\alpha\right\rangle \ .\end{aligned}$$

And, eventually, we obtain:

$$\rho^A = \sum_{k=1}^{d_B} p^A_k \left|\chi^A_k\right\rangle\!\left\langle\chi^A_k\right| \ , \tag{7}$$

where $\{\left|\chi_j\right\rangle\}_{j=1}^{d_B}$ is a set of d_B pure states on $\mathcal{H}_A$ which, usually, are nonorthogonal. This provides the following geometric quantum state, at fixed d_B:

$$\mu^A_{d_B}(dZ) := \sum_{k=1}^{d_B} p^B_k \delta_{\chi_k}(dZ) \ ,$$

where δ_{χ_k} is the Dirac measure with support only on the point $\chi_k \in \mathcal{P}(\mathcal{H}_A)$ corresponding to the ket $\left|\chi_k\right\rangle$.

While it is possible to track all information about $\left\{p^A_k\right\}_{k=1}^{d_B}$ for small d_B, in the thermodynamic limit this rapidly becomes infeasible. A probabilistic description becomes more appropriate. One could object that this is not a concern since, at each step in the limit, the spectral decomposition $\rho^A = \sum_{i=1}^{d_A} \lambda_i \left|\lambda_i\right\rangle \left\langle\lambda_i\right|$, where the λ_i are the Schmidt coefficients of $\left|\psi_{AB}\right\rangle$, is always available. However, this retains only ρ^A's matrix elements, erasing the information contained in the vectors $\left|v_j\right\rangle = \sqrt{p^A_j}\left|\chi^A_j\right\rangle$. That is, ρ^B has been erased from the description.

However, this information can be crucial to understanding A's behavior. The geometric formalism resolves this issue as it naturally keeps the "relevant" information by handling measures and probability distributions. In the limit of a large "environment" B, despite the fact that storing all information about the environment's details is exponential in B's size, the geometric quantum state's form (convex sum of Dirac deltas) facilitates working with smooth approximations of increasing accuracy. It does so by retaining the information about its "purifying environment".

Since we are interested here in the thermodynamics, one needs to operationally define the thermodynamic-limit procedure. We do so by confining ourselves to modular systems and defining an iterative procedure. Modular systems are those made by identical subsystems, each described by a Hilbert space $\mathcal{H}_d$ of dimension d. Thus, we imagine our system to contain N_A such repetitive units, while the environment contains $N_B \geq N_A$. This means $\mathcal{H}_A = \mathcal{H}_d^{\otimes N_A}$ and $\mathcal{H}_B = \mathcal{H}_d^{\otimes N_B}$, so that $d_A = d^{N_A}$ and $d_B = d^{N_B}$. At any given iteration, the joint system will always be in a pure state $\left|\psi_{AB}(N_B)\right\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$.

We also imagine that the system's global dynamics has a Hamiltonian H_{AB} of fixed functional form. For example, the XXZ model. Starting with $N_B = N_A$, at each step we add one repetitive unit $N_B \to N_B + 1$ and choose a series of pure states $\left\{\left|\psi_{AB}(N_B)\right\rangle\right\}_{N_B}$ with the required property that the limit of the average energy has to be finite:

$$\lim_{N_B \to \infty} \frac{\left\langle\psi_{AB}(N_B)\right| H_{AB} \left|\psi_{AB}(N_B)\right\rangle}{N_A + N_B} = \varepsilon \ .$$

For example, one can decide to consistently pick the ground state of the Hamiltonian H_{AB}. In general, though, there is no unique way of performing the procedure. However, with any specific choice of the series $\left\{\left|\psi_{AB}(N_B)\right\rangle\right\}_{N_B}$ satisfying the constraint on average energy, the procedure is well-defined, physical, and meaningful. It provides an operational way to study the thermodynamic limit of the geometric quantum state $\mu^A_{d_B}$.

That said, by no means does this guarantee the limit always exists. However, it does allow exploring it in a physically meaningful way. In particular, given this operational implementation of the thermodynamic limit, we say that:

$$\lim_{d_B \to \infty} \mu^A_{d_B} = \mu^A_\infty \ ,$$

This requires a geometric quantum state μ^A_∞ on $\mathcal{P}(\mathcal{H}_A)$ such that, for any $\epsilon > 0$ arbitrarily small, one can always find some finite $\overline{d}_B$ such that for any $d_B \geq \overline{d}_B$ one has that $D(\mu^A_{d_B}, \mu^A_\infty) \leq \epsilon$. Here, $D(\mu, \nu)$ is a notion of distance between geometric quantum states that we take to be the measure-theoretic counterpart of the total variation distance: $D(\mu, \nu) := \sup_{S \in \mathcal{B}} |\mu(S) - \nu(S)|$, where $\mathcal{B}$ is σ-algebra of $\mathcal{P}(\mathcal{H})$'s Borel sets.

When the limit exists, we say that the thermodynamic limit of the geometric quantum state is μ^A_∞ or, equivalently, P^A_∞:

$$\begin{aligned} P^A_\infty\left[\mathcal{O}\right] &= \int_{\mathcal{P}(\mathcal{H}_A)} \mu^A_\infty(dZ)\mathcal{O}(Z) \\ &= \sum_{k=1}^{\infty} p^A_k \mathcal{O}(\chi^A_k) \ . \end{aligned}$$

P^A_∞ is a functional whose operational meaning is understood in terms of ensemble theory, as explained above. Geometric quantum states describe ensembles of independent and noninteracting instances of the same quantum system whose pure states are distributed according to a given probability distribution. Loosely speaking, if we pick a random pure state out of the ensemble described by P^A_∞, the probability of finding it in a small region around Z is $dP_Z = \mu^A_\infty(dZ)$.

IV. FROM GEOMETRY TO STATISTICS

Several observations serve to motivate defining statistical mechanics using the geometric formalism. Consider a large system consisting of a macroscopic number M of qubits from which we extract, one by one, $\mathcal{N}$ qubit states. Describing small subsystems of a macroscopic quantum system places us in the realm of quantum statistical mechanics. It is therefore reasonable to assume that the qubit states are distributed according to Gibbs' canonical state $\gamma_\beta = e^{-\beta H}/Z_\beta$. This is statistically meaningful by means of ensemble theory and, thus, interpreted as a collection of identical noninteracting systems, each in an energy eigenstate, with relative frequency given by Boltzmann rule.

However, one can see how the assumption that all systems must be in one of the energy eigenstates can be relaxed. After we extract the k-th sample from the macroscopic system, that sample's state is supposed to be an energy eigenstate $\left|E_i^{(k)}\right\rangle$ with probability $p(Z(|E_i^{(k)}\rangle)) \propto e^{-\beta E_i^{(k)}}$. *A priori*, however, there is no reason to assume that the Hamiltonians H_k of all the samples are identical to each other. In fact, $\left|E_i^h\right\rangle \neq \left|E_i^k\right\rangle$ and $E_i^h \neq E_i^k$. Even if they are, in principle there is no reason why the qubits should be in their energy eigenstates. This point was originally made by Khinchin [29] and Schrödinger [30], who advocated for the use of ensembles of wave-functions.

To address this, a description of the system's state that does not contain this assumption is provided by the continuous counterpart of Gibbs canonical state, first introduced in Ref. [19], written as the following functional:

$$P_\beta[A] = \frac{1}{Q_\beta[h]} \int_{\mathcal{P}(\mathcal{H})} e^{-\beta h(Z)} A(Z) dV_{FS} \ ,$$

where:

$$Q_\beta[h] = \int_{\mathcal{P}(\mathcal{H})} e^{-\beta h(Z)} dV_{FS} ~,$$

with $h(Z) = \sum_{\alpha\beta} H_{\alpha\beta} Z^\beta \overline{Z}^\alpha$. While this distribution retains a characteristic feature of the canonical Gibbs ensemble:

$$\frac{p_\beta\big(Z(|E_n\rangle)\big)}{p_\beta\big(Z(|E_m\rangle)\big)} = e^{-\beta(E_n-E_m)} ~,$$

it also extends this "Boltzmann" rule to arbitrary states:

$$-\log\left[\frac{p_\beta\big(Z(|\psi\rangle)\big)}{p_\beta\big(Z(|\phi\rangle)\big)}\right] = \beta\left[h(Z(\psi)) - h(Z(\phi))\right] ~.$$

Therefore, formulating the statistical mechanics of quantum states via the geometric formalism differs from the standard development, based on an algebraic formalism. This becomes obvious when we write the Gibbs canonical density matrix γ_β in the geometric formalism:

$$\begin{aligned} p_{\text{Gibbs}}(Z) &= \sum_{k=0}^{D-1} \frac{e^{-\beta E_k}}{\operatorname{Tr} e^{-\beta H}} \delta[Z - Z(|E_k\rangle)] \\ &\neq \frac{e^{-\beta h(Z)}}{Q_\beta[h]} ~. \end{aligned}$$

This makes explicit the standard formalism's assumption that the measure is Dirac-like—peaked on energy eigenstates.

Despite quantum statistical mechanics' undeniable successes, this assumption is not, in general, justified. In point of fact, it is the origin of the missing environmental information noted above. These arguments motivate an alternative formulation of the statistical mechanics of quantum systems, first introduced in Ref. [19]—one based on geometric quantum states rather than on the familiar density matrices.

V. STATISTICAL TREATMENT OF GEOMETRIC QUANTUM MECHANICS

Representing a quantum system's state as a continuous mixed state was first broached, to our knowledge, by Brody and Hughston [19, 20]. Our goal here is to advance the idea, going from statistical mechanics to thermodynamics. To set the stage for a *geometric quantum thermodynamics*, the following first presents our version of their results, derived via the formalism defined in Sec. III, and then expands on them. We begin with the fundamental postulate of classical statistical mechanics and its adaptation to quantum mechanics—the microcanonical and canonical ensembles.

A. Classical microcanonical ensemble: A priori equal probability

At its most basic level, the fundamental postulate of classical statistical mechanics is that, in an isolated system's phase space, *microstates with equal energy have the same chance of being populated.* Calling $\vec{q}$ and $\vec{p}$ generalized velocities and positions, which provide a coordinate frame for the classical phase-space, the postulate corresponds to assuming that the *microcanonical* probability distribution P_{mc} of finding the system in a microstate $(\vec{p},\vec{q})$ is, at equilibrium:

$$P_{\text{mc}}(\vec{q},\vec{p}) = \begin{cases} 1/W(\mathcal{E}) & \text{if } E(\vec{q},\vec{p}) \in [\mathcal{E}, \mathcal{E}+\delta\mathcal{E}] \\ 0 & \text{otherwise} \end{cases} ~.$$

Here, $W(\mathcal{E})$ is the number of microstates $(\vec{q},\vec{p})$ belonging to energy shell $I_{\text{mc}} \coloneqq [\mathcal{E}, \mathcal{E}+\delta\mathcal{E}]$:

$$W(\mathcal{E}) = \int_{E(\vec{q},\vec{p})\in I_{\text{mc}}} d\vec{q} \wedge d\vec{p} ~,$$

with $\int d\vec{q} \wedge d\vec{p} ~ P_{\text{mc}}(\vec{q},\vec{p}) = 1$.

B. Quantum microcanonical ensemble: A priori equal probability

Quantum statistical mechanics relies on the quantum version of the Gibbs ensemble. For macroscopic isolated systems this is usually interpreted as the quantum system having equal chance p_{mc} to be in any one of the energy eigenstates $|E_n\rangle$, as long as $E_n \in I_{\text{mc}}$:

$$p_{\text{mc}}(E_n) = \begin{cases} 1/\mathrm{W}_{\text{mc}} & \text{if} E_n \in [\mathcal{E}, \mathcal{E}+\delta\mathcal{E}] \\ 0 & \text{otherwise} \end{cases} ~.$$

Here, $W_{\text{mc}} = \sum_{E_n \in I_{\text{mc}}} 1$ is the number of energy eigenstates that belong to the microcanonical window I_{mc}. Thus, the equal-probability postulate provides the following definition for the microcanonical density matrix:

$$\rho_{\text{mc}} = \frac{1}{W_{\text{mc}}} \sum_{E_n \in I_{\text{mc}}} |E_n\rangle \langle E_n| ~.$$

Geometric quantum mechanics gives an alternative way to extend equal-probability to quantum systems, which we discuss now.

C. Geometric quantum microcanonical ensemble: A priori equal probability

The following summarizes an approach to the statistical mechanics of quantum systems first presented in Refs. [19, 20, 22]. In geometric quantum mechanics the role of the Hamiltonian operator as the generator of unitary dynamics is played by the real quadratic function:

$$h(Z) = \sum_{\alpha\beta} H_{\alpha\beta} Z^\alpha \overline{Z}^\beta ~,$$

where $H_{\alpha\beta}$ are the matrix elements of the Hamiltonian operator in a reference basis; see Eq. (3). As h is the generator of Liouville dynamics on the pure-state manifold $\mathcal{P}(\mathcal{H})$, it is easy to see that there is a straightforward geometric implementation of the a-priori-equal-probability postulate in the quantum setting:

$$p_{\mathrm{mc}}(Z) = \begin{cases} 1/\Omega(\mathcal{E}) & h(Z) \in I_{\mathrm{mc}}, \text{ for all } Z \in \mathcal{P}(\mathcal{H}) \\ 0 & \text{otherwise} \end{cases} ~.$$

Due to normalization, $\Omega(\mathcal{E})$ is the volume of the quantum-state manifold enclosed by the microcanonical energy shell I_{mc}:

$$\Omega(\mathcal{E}) = \int_{h(Z) \in I_{\mathrm{mc}}} dV_{FS} ~.$$

where dV_{FS} is the Fubini-Study volume element introduced in Sec. II. In probability-and-phase coordinate $Z^\alpha = \sqrt{p_\alpha} e^{i\nu_\alpha}$ the volume element has the explicit form:

$$dV_{FS} = \prod_{\alpha=1}^{n} \frac{dp_\alpha d\nu_\alpha}{2} ~.$$

Following Heslot [4], we introduce dimensional coordinates via:

$$Z^\alpha = \frac{X^\alpha + iY^\alpha}{\sqrt{\hbar}} ~,$$

where X^α and Y^α are real numbers with dimensions $[X] = \left[\sqrt{\hbar}\right] = \text{Length}\sqrt{\text{Mass/Time}}$ and $[Y] = \left[\sqrt{\hbar}\right] = \text{Momentum}\sqrt{\text{Time/Mass}}$. The ratio X/Y is a pure number, while their product XY has the dimension $\hbar$ of an action. Note that $dp_\alpha d\nu_\alpha/2 = dX_\alpha dY_\alpha/\hbar$. This allows us to write the Fubini-Study measure in a classical fashion:

$$\begin{aligned} dV_{FS} &= \prod_{\alpha=1}^{D-1} \frac{dX^\alpha dY^\alpha}{\hbar} \\ &= \frac{d\vec{X} d\vec{Y}}{\hbar^{D-1}} ~, \end{aligned}$$

where the X^α play the role of generalized coordinates and Y^α that of generalized momenta. However, it is worth noting that the global geometry of the classical phase-space differs substantially from that of $\mathcal{P}(\mathcal{H})$.

Given these definitions, it is now possible to calculate the number of states $\Omega(\mathcal{E}) \approx \omega(\mathcal{E})\delta\mathcal{E}$, where $\delta\mathcal{E}$ is the size of the microcanonical energy shell and $\omega(\mathcal{E})$ is the density of states:

$$\begin{aligned} \omega(\mathcal{E}) &= \int_{h(Z)=\mathcal{E}} dV_{FS} \\ &= \frac{\pi^{D-1}}{(D-1)!} \sum_{k=0}^{D-1} \prod_{j\neq k, j=0}^{D-1} \frac{(\mathcal{E} - E_k)_+}{(E_j - E_k)} ~, \end{aligned}$$

where $(x)_+ := \max(0, x)$. Since $\mathcal{E} \in [E_0, E_{\max}]$, there exists an $\overline{n}$ such that $\mathcal{E} \in]E_{\overline{n}}, E_{\overline{n}+1}[$. This means that we can stop the sum at $k = \overline{n}(\mathcal{E})$ since for all $k > \overline{n}$ we have $(\mathcal{E} - E_k)_+ = 0$. This gives:

$$\omega(\mathcal{E}) = \frac{\pi^{D-1}}{(D-1)!} \sum_{k=0}^{\overline{n}(\mathcal{E})} \frac{(D-1)(\mathcal{E} - E_k)^{D-2}}{\prod_{j\neq k, j=0}^{D-1} (E_j - E_k)} ~. \tag{8}$$

This is in agreement with Ref. [20]'s Eq. (5). Appendix B 3 provides a detailed proof, using a convenient mathematical result by Ref. [31].

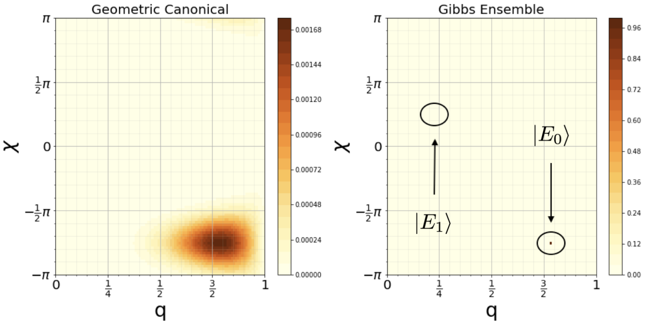


Figure 1. Alternate ensembles in the geometric and standard settings: Differences are plainly evident. Canonical probability distributions on a qubit's state manifold $\mathbb{C}P^1$ with coordinates $Z = (Z^0, Z^1) = (\sqrt{1-q}, \sqrt{q}e^{i\chi})$ where $q \in [0, 1]$ and $\chi \in [-\pi, \pi]$. $\mathbb{C}P^1$ discretized using a 100-by-100 grid on the (q, χ) coordinates exploiting the fact that, with these coordinates, the Fubini-Study measure is directly proportional to the Cartesian volume element $dV_{FS} = dqd\chi/2$. The Hamiltonian is $H = \sigma_x + \sigma_y + \sigma_z$, with $\hbar = 1$ and inverse temperature $\beta = 5$ ($k_{\mathrm{B}} = 1$). (Right) Gibbs ensemble where circles enclose the positions around the coordinates of the respective eigenvectors $\big(q(|E_0\rangle), \chi(|E_0\rangle)\big) = (0.789, -2.356)$ and $\big(q(|E_1\rangle), \chi(|E_1\rangle)\big) = (0.211, 0.785)$. (Left) Geometric Canonical Ensemble.

D. Quantum canonical ensemble: Statistical physics of quantum states

The geometric approach to microcanonical ensembles extends straightforwardly to the canonical case, defining the continuous canonical ensemble as:

$$p_\beta(Z) = \frac{e^{-\beta h(Z)}}{Q_\beta[h]} ~, \tag{9}$$

where:

$$Q_\beta[h] = \int_{\mathcal{P}(\mathcal{H})} e^{-\beta h(Z)} dV_{FS} ~.$$

Reference [19] first proposed the general form of the canonical partition function $Q_\beta[h]$, working it out explicitly in several low-dimensional cases. Follow-on work provided an exact formula valid for arbitrary finite-dimensional Hilbert spaces [20]. Appendix B 3 provides an alternative proof and explicit examples of:

$$Q_\beta[h] = \sum_{k=0}^{D-1} \frac{e^{-\beta E_k}}{\prod_{j=0, j\neq k}^{n} (\beta E_k - \beta E_j)} ~. \tag{10}$$

This is in full agreement with Ref. [20]'s Eq. (6).

With the ensembles laid out we can now see the emergence of geometric quantum thermodynamics, with its fundamental laws.

VI. GEOMETRIC QUANTUM THERMODYNAMICS

With a consistent statistical geometric quantum mechanics in hand, we can now formulate geometric quantum thermodynamics. This is modeled via the geometric canonical state Eq. (9). Notice that, in this setting, an appropriate entropy definition has yet to be given. Paralleling early work by Gibbs, one can consider the functional:

$$H_q\left[p\right] = -k_{\mathrm{B}} \int_{\mathcal{P}(\mathcal{H})} p(Z) \log p(Z) dV_{FS} ~.$$

An information-theoretic analysis of this quantity and its relation with the von Neumann entropy was done in Ref. [32]. This functional allows properly evaluating $p(Z)$'s entropy if and only if the dimension of the support of p has the same real dimension of $\mathbb{C}P^n$. Reference [33] defined and explored the appropriate generalization to geometric quantum states with generic support, including fractal distributions.

Let's consider H_q's role, though, for the quantum foundations of thermodynamics. For Eq. (9)'s geometric canonical ensemble this gives:

$$H_q = \beta(U - F) ~,$$

where:

$$U := \int_{\mathcal{P}(\mathcal{H})} p_\beta(Z) h(Z) dV_{FS} \quad \text{and}$$
$$F := -\frac{1}{\beta} \log Q_\beta$$

are, respectively, the average energy and the free energy arising from the geometric partition function Q_β.

This means that we can directly import a series of fundamental results from classical thermodynamics and statistical mechanics into the quantum setting, fully amortizing the effort invested to develop the geometric formalism.

A. First Law

The first result is a straightforward derivation of the First Law:

$$\begin{aligned} dU &= \int_{\mathcal{P}(\mathcal{H})} dV_{FS} p(Z) dh(Z) + \int_{\mathcal{P}(\mathcal{H})} dV_{FS} dp(Z) h(Z) \\ &= dW + dQ ~. \end{aligned} \tag{11}$$

We call the contribution dW *work*, since it arises from a change in the Hamiltonian $h(Z)$ generated by an external control operating on the system. We call the contribution dQ *heat*, as it is associated with a change in entropy. Indeed, by direct computation one sees that:

$$dH_q = \beta dQ \qquad \text{and} \qquad dF = dW ~.$$

This gives the standard form of the First Law for isothermal, quasi-static processes:

$$dU = T dH_q + dF ~,$$

where $T := (k_{\mathrm{B}}\beta)^{-1}$. Conforming to the conventional statistical approach to thermodynamics, beyond energy conservation, one can use the First Law to extract phenomenological relations (e.g., Maxwell's relation) that hold at thermodynamic equilibrium: $\partial U / \partial H_q = T$. In this, the partial derivatives are intended as infinitesimal changes occurring while maintaining the system at thermal equilibrium.

B. Second Law

The Second Law follows from the Crooks [34] and Jarzynski [35] fluctuation theorems [26, 36, 37]. Their treatment can be straightforwardly exploited, thanks to the Hamiltonian nature of Schrödinger's equation when written on the quantum-state manifold $\mathcal{P}(\mathcal{H})$.

As summarized in Eq. (3), given a Hamiltonian $h(Z,\lambda)$ on $\mathcal{P}(\mathcal{H})$ that depends on an externally-controlled parameter $\lambda = \lambda(t)$, the unitary evolution is given by the Liouville equation Eq. (3) as in classical mechanics:

$$\frac{\partial p(Z)}{\partial t} = \left\{ p(Z), h(Z,\lambda) \right\} ~.$$

Notably, one can apply Jarzynski's original argument [38] to driven quantum systems, without the need to exploit the *two-times measurement scheme* [26]. The setup is standard.

The ensemble of quantum systems starts in a geometric canonical state defined by Eq. (9) and is then driven with a Hamiltonian that depends on a parameter λ following the time-dependent protocol $\lambda = \lambda(t)$ with $t \in [0, 1]$. This leads directly to an ensemble of protocol realizations. That said, we define the *single-trajectory work* as:

$$W = \int_0^1 \dot{\lambda}(t) \frac{\partial h}{\partial \lambda}\big(Z(\psi_t), \lambda(t)\big) dt \ ,$$

where $\dot{\lambda} = d\lambda/dt$ and $Z(\psi_t)$ are the homogeneous coordinates on $\mathbb{C}P^{D-1}$ for $|\psi_t\rangle$. Therefore, $|\psi_t\rangle$ are the solutions of Eq. (4).

With these premises, Jarzynski's original argument applies *mutatis mutandis* to give:

$$\begin{aligned} \left\langle e^{-\beta W} \right\rangle_{\text{ens}} &= \frac{Q_\beta[h(\lambda_f)]}{Q_\beta[h(\lambda_i)]} \\ &= e^{-\Delta F} \ , \end{aligned} \tag{12}$$

where $\lambda(0) = \lambda_i$ and $\lambda(1) = \lambda_f$ and $\langle x \rangle_{\text{ens}}$ denotes the ensemble average over many protocol realizations. From this, one directly applies Jensen's inequality:

$$\left\langle e^{-\beta W} \right\rangle_{\text{ens}} \geq e^{-\beta \langle W \rangle}_{\text{ens}}$$

to obtain the Second Law's familiar form:

$$\langle W \rangle_{\text{ens}} \geq F \ . \tag{13}$$

VII. GEOMETRIC THERMALIZATION IN A PHENOMENOLOGICAL MODEL

The validity of geometric quantum thermodynamics, as defined above, hinges on the assumption of (geometric) thermal equilibrium. It therefore implicitly relies on a dynamical mechanism driving the system towards the geometric canonical ensemble. This section shows that this occurs in at least one model for the out-of-equilibrium dynamics of a single qubit.

A quantum system interacting with its surroundings evolves in a nonunitary fashion due to the fact that it exchanges energy (or other extensive quantities) and so becomes correlated with its environment. This can be modeled using the theory of open quantum systems and its dissipative dynamics [39–42]. While most approaches focus on establishing an equation governing the dynamical evolution of the system's density matrix, here we are interested in the thermodynamics of the geometric quantum state as the ensemble behind the density matrix. A principled description and modeling of the dynamics of an open quantum system within the geometric approach is beyond the present scope. Though, its development is currently ongoing.

Instead, the following shows how to represent dissipation within the geometric formalism for a stochastic model. This serves a twofold purpose. First, it provides simple examples of how geometric quantum mechanics evolves open quantum systems in a variety of cases. Second, it supports the theory developed above with a numeric analysis of an experimentally relevant scenario.

While the emphasis is still on the geometric formalism, and its natural phase-space geometry, this approach is not far from "Stochastic Schrodinger Equations". See, for example, Refs. [39, 43–46]) that import techniques from the classical theory of stochastic processes. The following exploits this idea, applying it to the geometric language and drawing from a variety of known approaches. It does so by examining a phenomenological model for dissipative dynamics that, as we show, exhibits thermalization towards the geometric canonical ensemble.

It considers the stochastic dynamics of a two-level system with state space $\mathcal{P}(\mathcal{H}) \sim \mathbb{C}P^1$. Generally, this results from a two-state approximation of a more complex system interacting with an environment. It gives a standard approximation that provides sensible results in a variety of physical regimes. These include systems that inherently consist of two states, such as spin-1/2, chiral molecules [47–53], and atoms at low temperature, considering only the two lowest states. They also include, though, continuous-variable systems in a double-well potential, Josephson junctions [54], and effective descriptions of macroscopic condensates. As a related technical aside beyond quantum mechanics, we note that the proper analysis and simulation of stochastic dynamics on Riemannian manifolds is a topic of its own interest [55, 56].

Accounting for the nonisolated nature of the system involves modeling the environment and the latter's effect on the effective qubit. This, therefore, depends on the specific case under study and leads to different effective equations governing the qubit's nonequilibrium behavior. From the system's perspective, however, a general setup is available in a regime in which coupling with the environment is weak and the environment is effectively large and disordered. These approximations are expected to hold for large environments, where one can argue for the emergence of stochastic dynamics for the evolution of the open system.

The prototypical case, in which a specific form of these equations can be derived by integrating out the environmental degrees of freedom, is given by the Caldeira-Leggett model [57–59] with an environment modeled by an infinite number of noninteracting harmonic oscillators. Respecting these approximations' validity, a generic model of Langevin-like dynamics on $\mathbb{C}P^1$ is:

$$\begin{aligned} \dot{p} &= -\partial_\phi E + V_p + W_p \ , \\ \dot{\phi} &= \partial_p E + V_\phi + W_\phi \ , \end{aligned} \tag{14}$$

in (p, ϕ) coordinates. In this, $E = E(p, \phi)$ is an effective Hamiltonian generating the deterministic part of the dynamics; see Eq. (4). This is a renormalized version of the system's Hamiltonian. V_p and V_ϕ depend linearly on (p,ϕ) and $(\dot{p},\dot{\phi})$. They describe (i) dissipative mechanisms such as friction, modeled with a dependence on $\dot{p}$ or $\dot{\phi}$, as in standard Langevin equations, and (ii) unstable states, modeled with a dependence $V_p = -kp$ to allow for exponential decay $p_{\mathrm{decay}}(t) \sim p_0 e^{-kt}$, as in a two-level atom decaying into its ground state.

Finally, W_p and W_ϕ are stochastic variables with no drift that account for the environment's mixing effect on the system. When the environment is sufficiently large and unstructured, they can be modeled as Gaussian processes, $\mathbb{E}[W_a(s+t)W_b(s)] = \mathbb{E}[W_a(t)W_b(0)] \approx \delta_{ab}\gamma_a\delta(t)$, with $a,b \in \{p,\phi\}$ and $\gamma_a \propto k_{\mathrm{B}}T$, with T the temperature of the environment. This is true in the Caldeira-Leggett model for Ohmic baths.

As anticipated above, specific forms of these equations have successfully modeled the evolution of a variety of two-level systems. We also note how, in several cases, and also in Refs. [60–64], this approach to open quantum systems is quite similar to GQM as it relies on canonical representations of the quantum state space. For chiral molecules, for example, one has $E(p,\phi) = \delta \langle\sigma_x\rangle + \epsilon \langle\sigma_z\rangle = \delta 2\sqrt{p(1-p)}\cos\phi + \epsilon(1-2p)$, $V_p = -k\dot{p}$, with $k \sim 10^{-1}$, $W_\phi = V_\phi = 0$ and $W_p(t)$ white noise with strength $\gamma_p \propto k_{\mathrm{B}}T$. The thermodynamics arising from this set of dynamical equations has been studied in detail [47–53]. The goal here is rather to showcase the experimental relevance of the geometric canonical ensemble. The following does so showing, numerically, that the evolution provided by the stochastic equations above leads to the dynamical emergence of the geometric canonical ensemble. This is directly relevant to the out-of-equilibrium dynamics of an ensemble of chiral molecules or of an ensemble of experiments with Josephson junctions.

The specific stochastic equations under study are:

$$\begin{aligned} \dot{p} &= \delta 2\sqrt{p(1-p)}\sin\phi - k_d p - k_f\dot{\phi} + \sqrt{\gamma}\xi(t) \\ \dot{\phi} &= -\delta\frac{1-2p}{\sqrt{p(1-p)}}\cos\phi + 2\epsilon\ , \end{aligned} \tag{15}$$

where k_d and k_f are coefficients accounting for dissipation mechanisms, such as instability of a state and friction. Up to simple re-definition of variables, that does not change the physics, the model with $k_d = 0$ is the same as in Ref. [49, 50].

Exploiting the Markovian character of Gaussian noise, the statistics of many independent realizations of this stochastic process on $\mathbb{C}P^1$ can be extracted by examining the time-aggregated statistics of a single, very long, trajectory. We thus simulate the long-time dynamics of a qubit initiated in a fully out-of-equilibrium configuration $q_0(p,\phi) = \delta(p-p_0)\delta(\phi-\phi_0)$, corresponding to a pure state $|p_0,\phi_0\rangle = \sqrt{1-p_0}\,|0\rangle + \sqrt{p_0}e^{i\phi_0}\,|1\rangle$, where $|0\rangle, |1\rangle$ are the standard computational basis. For chiral molecules, these are the (left and right) chiral eigenstates. Here, we show the results for $p_0 = 0.9$ and $\phi = 4\pi/3$ and checked that they do not depend on this choice. Results are shown for parameter values $\delta = \epsilon = 1$, $\gamma = 0.2$, and $k_d = 0$. While these match the model in Ref. [49, 50], the results are largely independent of this specific choice and hold for broad regimes in $(\delta,\epsilon,k_d,\gamma)$ parameter space.

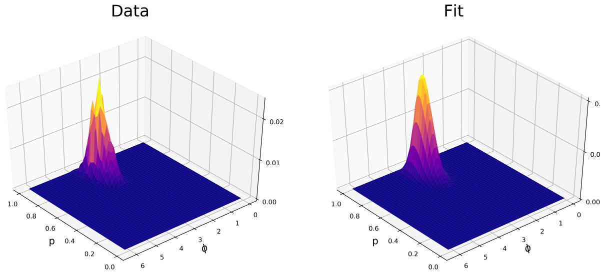
The analysis was performed as follows. After generating a single long-time trajectory using the Milstein method, we collected statistics $\tilde{P}_{nk}$. We then generated a histogram to approximate the probability that, at any given time, the system is found in a small region of the state space $\tilde{P}_{nk} \approx \overline{\Pr}[Z \in \mathcal{I}_{nk}] = \lim_{T\to\infty}\int_0^T\int_{\mathcal{I}_{nk}} q_t(Z)dV_{FS}$. In this, $\{\mathcal{I}_{nk}\}_{n,k=1}^N$ is a coarse graining of $\mathbb{C}P^1$ in which each region $\mathcal{I}_{nk} = [p_n,p_{n+1}] \times [\phi_k,\phi_{k+1}]$ has the same Fubini-Study volume $\mu_{FS}(\mathcal{I}_{nk}) = N^{-2}$, $p_k = n/N$, and $\phi_k = 2\pi k/N$. Reference [33] gives a detailed analysis of why this is an appropriate coarse-graining, its information-theoretic relevance, and how to generalize it to arbitrary $\mathbb{C}P^n$.

Concretely, the numerical analysis used $N = 50$. The dynamics was generated setting $T = 10^2$ in units in which $\hbar = \delta = 1$. This was chosen by numerically checking that the reconstructed histogram does not change significantly when increasing T. The time window $[0,T]$ was discretized to use the Milstein algorithm to generate Gaussian noise with $dt = 10^{-4}$. These, again, are consistent with the choices in Refs. [49, 50]. In short, the number of time steps $N_T = 10^6$, with $N_T dt = T$.

To extract the inverse temperature β the collected statistics were used to perform a 2D least-square fit to the geometric canonical ensemble. The latter's appropriateness was established by using the following figure of merit: $f = \sum_{n,k}|\tilde{P}_{nk} - q^{\mathrm{fit}}_{nk}|^2 \in [0,1]$, where $q^{\mathrm{fit}}_{nk} = Q^{-1}\beta^*\int_{\mathcal{I}_{nk}} dV_{FS}e^{-\beta^* E(Z)}$ and β^* is the optimal value extracted from the least-square fit. This is the total variation distance between the coarse-grained geometric quantum states obtained from the data $\left\{\tilde{P}_{nk}\right\}_{n,k}$ and the one obtained from the best fit to the geometric canonical ensemble $\left\{q^{\mathrm{fit}}_{nk}\right\}_{n,k}$. It ranges from zero to one and is the classical analog of the well-known trace-distance for density matrices. At selected parameters, $f \approx 5.6 \times 10^{-4}$. This quantifies the visually excellent agreement seen in Fig. 2.

Before drawing broad conclusions, a few comments are in order regarding specific results. First, thermalization is observed even when changing parameter values. This is true for *any* of the Hamiltonian parameters, δ and ϵ. Moreover, there are good numerical indications that this holds for any $k_d > 0$. However, k_d and γ do affect the effective (inverse) temperature β^* the system reaches. Analyzing how this happens and the underlying mechanisms is beyond the present scope, which aimed only at establishing the predictive relevance of the geometric canonical ensemble in an experimentally realistic settings.

Second, we ignored issues related to the time-scale at which the aggregated geometric quantum state reaches the canonical form. These were bypassed by using a time window $[0,T]$ that guaranteed the aggregated data does not change when increasing T.



Data

Fit

Figure 2. Comparing time-aggregated data of a single trajectory generated by Eq. (15)'s stochastic model (left) to the fit to a geometric canonical ensemble with functional form as in Eq. (9) (right). Here, $h(Z) = E(p, \phi) = \delta \langle \sigma_x \rangle + \epsilon \langle \sigma_z \rangle = \delta 2\sqrt{p(1-p)} \cos\phi + \epsilon(1-2p)$, with $\delta = \epsilon = 1$. The excellent agreement is visually clear and quantified by a total variation distance between the two distributions of $f \approx 5.6 \times 10^{-4}$.

Third, Eq. (15)'s model arises from a bath that is a set of noninteracting harmonic oscillators with Ohmic correlation functions and interactions linear in the phase difference ϕ, leading to a friction $\propto \dot{\phi}$. A different kind of interaction is possible, linear in the population p, that leads to a friction term $\dot{p}$. While not reported here, there are numerical indications that this alternative exhibits thermalization to the geometric canonical ensemble as well. This supports the intuition that thermalization is mostly driven by the lack of memory of the stochastic term, ultimately due to the Ohmic nature of the bath's correlation functions.

Fourth, the effective nature of the description makes the model widely applicable. And so, a number of straightforward generalizations would be quite interesting to explore. These include, for example, changing the noise structure to accommodate limited memory and allowing for competition between the different ways in which the system interacts with the harmonic bath and the decay in both p and ϕ. Of particular interest, both conceptually and practically, is determining which terms lead to dynamical localization and what kinds of system-bath interactions are necessary for these terms to emerge by integrating out the bath degrees of freedom.

VIII. SUMMARY AND CONCLUSION

While historically quantum mechanics is firmly rooted in an algebraic formalism, an alternative based on the differential geometry of quantum state space $\mathcal{P}(\mathcal{H}) \sim \mathbb{C}P^{D-1}$ is readily available.

As previous works repeatedly emphasized [1, 4, 10], the geometric approach brings quantum and classical mechanics much closer, aiming to leverage the best of both. The space $\mathcal{P}(\mathcal{H})$ of quantum states is a Kähler space, with two intertwined notions of geometry—Riemannian and symplectic. It also sports a preferred notion of measure, selected by invariance under unitary transformations—the Fubini-Study measure. One can exploit this rich geometric structure to define generic probability measures on $\mathcal{P}(\mathcal{H})$. The result is a new kind of quantum state—the *geometric quantum state* [27]—that generalizes the familiar density matrix but provides more information about a quantum system's physical configuration. Essentially, it expresses the multitude of ensembles, induced by different environments, behind a density matrix.

Leveraging parallels between the geometric formalism and classical mechanics, the statistical treatment of geometric quantum mechanics provides a continuous counterpart of Gibbs ensembles. Section VI laid out how to establish quantum thermodynamics on the basis of the geometric formalism. Building on Section V's statistical treatment of geometric quantum mechanics, it derived the First and Second Laws of Geometric Quantum Thermodynamics. Despite the two results appearing identical to the existing laws, derived within standard quantum statistical mechanics, they involve quantities that are genuinely different. Understanding how Eqs. (11), (12), and (13) connect to their standard counterparts [26] is a challenge that we must leave for the future. We note Ref. [65] obtained a similar result that, lacking the geometric perspective, considered microcanonical and canonical ensembles of pure states, as first advocated by Khinchin [29] and Schrödinger [30].

Remarkably, predictions from standard quantum statistical mechanics and its geometric counterpart differ. This poses a challenge: Which theory should one use? Ultimately, this problem does not have a generic solution. Answering the question requires understanding the details of the long-time dynamic of an open quantum system and, in general, this will be be model-specific. Here, to showcase the relevance of the geometric approach, we showed that there is a class of known stochastic models, aimed at describing chiral molecules and Josephson's junctions, that indeed does exhibit dynamical evolution towards the geometric canonical ensemble. One thus expects the predictions from geometric quantum thermodynamics to hold in the cases where the dynamical model in Eq. (15) is justified.

The geometric approach to quantum thermodynamics opens the door to new and interesting questions and novel research avenues. Let's mention two. First, the ensemble interpretation of geometric quantum mechanics suggests employing the geometric formalism to describe the thermodynamics of ensembles, rather than relying on that of density matrices. The main advantage is that this delineates the environmental resources required to support a given density matrix. Indeed, while two different experimental setups can give rise to the same density matrix, their difference implicitly lies in the distinct ways the density matrix is created. This is directly relevant to the energetics of information processing technologies built from quantum computers and quantum sensors.

Second, from a conceptual perspective, geometric quantum thermodynamics and statistical mechanics are as at least as powerful as their standard counterpart. Yet, they can make different predictions. Self-consistency of thermodynamic predictions suggests that this difference should be negligible in a truly macroscopic regime in which both system and environment are macroscopically large. This is, however, a highly nontrivial statement whose proof requires a much better understanding of the emergence of thermodynamic predictions from fully dynamical considerations. We believe the new research avenues, together with the larger perspective provided by geometric quantum mechanics, will greatly enrich our understanding of the phenomenology of many-body quantum systems.

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DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding authors upon reasonable request.

Appendix A: Independent result

For completeness, the following summarizes Ref. [31]'s result called on in calculating the density of states. Given the n-simplex $\Delta_n : \left\{ \vec{x} \in \mathbb{R}^n_+ \ : \vec{e} \cdot \vec{x} \leq 1 \right\}$, where $\vec{e}$ is the vector of ones in $\mathbb{R}^n$, a section of the simplex is defined by a vector $\vec{a} \in \mathbb{S}^n$ and we want to compute the n-dimensional and $(n-1)$-dimensional volume of the following sets:

$$\begin{aligned} \Theta(\vec{a}, t) &:= \Delta_n \cap \left\{ \vec{x} \in \mathbb{R}^n : \vec{a}^T \cdot \vec{x} \leq t \right\} \text{ and} \\ S(\vec{a}, t) &:= \Delta_n \cap \left\{ \vec{x} \in \mathbb{R}^n : \vec{a}^T \cdot \vec{x} = t \right\} \ , \end{aligned}$$

where $\vec{a}^T$ is the transpose of $\vec{a}$. The result assumes flat geometry, which is obtained from the volume element $dp_1 dp_2 \ldots dp_n$. Letting $(x)_+ := \max(0, x)$ and $a_0 = 0$, then:

$$\begin{aligned} \mathrm{Vol}\left(\Theta(\vec{a}, t)\right) &= \frac{1}{n!} \sum_{k=0}^{n} \frac{(t - a_k)_+^n}{\prod_{j \neq k\,,\, j=0}^{n} (a_j - a_k)} \\ &= \frac{1}{n!} \frac{t^n}{\prod_{k=1}^{n} a_k} + \frac{1}{n!} \sum_{k=1}^{n} \frac{(t - a_j)_+^n}{\prod_{j \neq k\,,\, j=0}^{n} (a_j - a_k)} \end{aligned}$$

and:

$$\begin{aligned} \mathrm{Vol}\left(S(\vec{a}, t)\right) &= \frac{1}{(n-1)!} \sum_{k=0}^{n} \frac{(t - a_k)_+^{n-1}}{\prod_{j \neq k\,,\, j=0}^{n} (a_j - a_k)} \\ &= \frac{1}{(n-1)!} \frac{t^{n-1}}{\prod_{k=1}^{n} a_k} \\ &\quad + \frac{1}{(n-1)!} \sum_{k=1}^{n} \frac{(t - a_j)_+^{n-1}}{\prod_{j \neq k\,,\, j=0}^{n} (a_j - a_k)} \ . \end{aligned}$$

Appendix B: Geometric Quantum Density of States and Canonical Ensemble

Again for completeness, we first recall the basic definitions, given in the main text, used in the two sections that follow to calculate the density of states and statistical physics of quantum states in the geometric formalism.

1. Setup and notation

Consider a Hilbert space $\mathcal{H}$ of finite-dimension D. The manifold $\mathcal{P}(\mathcal{H})$ of states is the complex projective space $\mathbb{C}P^{D-1}$. A point Z on the manifold is a set of D homogeneous and complex coordinates $\{Z^\alpha\}$. A point corresponds to a pure state with the identification $Z \leftrightarrow \left|\psi\right\rangle = \sum_{\alpha=0}^{D-1} Z^\alpha \left|e_\alpha\right\rangle$, where $\left\{\left|e_\alpha\right\rangle\right\}_\alpha$ is an arbitrary but fixed basis of $\mathcal{H}$. This parametrization underlies the choice of a reference basis that, however, is ultimately irrelevant. While concrete calculations of experimentally measurable quantities can be made easier or harder by an appropriate coordinate system, the overall result is independent on such choices. The quantum mechanical expectation value is a quadratic and real function on the manifold of the quantum states:

$$\begin{aligned} a(Z) &:= \left\langle \psi(Z) \right| A \left| \psi(Z) \right\rangle \\ &= \sum_{\alpha, \beta = 0}^{D-1} A_{\alpha, \beta} Z^\alpha \overline{Z}^\beta \ . \end{aligned}$$

When $A = H$ is the system's Hamiltonian, the function $a(Z) = h(Z)$ generates the vector field V_H on $\mathbb{C}P^{D-1}$. The associated Hamiltonian equations of motion become the Schrödinger equation (and its complex conjugate) when using the standard formalism with Hilbert spaces. In the geometric formalism, states are functionals from the algebra of observables to the real numbers. Effectively, they are probability distributions, both discrete and continuous, on the quantum-state manifold $\mathbb{C}P^{D-1}$.

2. Microcanonical density of states: Proof of Eq. (8)

We start with the a priori equal probability postulate and build the microcanonical shell as follows:

$$p_{\mathrm{mc}}(Z) = \begin{cases} 1/W(\mathcal{E}) & \text{if } h(Z) \in [\mathcal{E}, \mathcal{E}+\delta\mathcal{E}] \\ 0 & \text{otherwise} \end{cases} .$$

Due to normalization we have:

$$W(\mathcal{E}) = \int_{h(z)\in I_{\mathrm{mc}}} dV_{FS} \ ,$$

where dV_{FS} is the volume element of the Fubini-Study metric:

$$dV_{FS} = \frac{1}{2^n} dp_1 dp_2 \ldots dp_n d\nu_1 \ldots d\nu_n \ .$$

This gives the manifold volume:

$$\mathrm{Vol}(\mathbb{C}P^n) = \frac{\pi^n}{n!} \ .$$

For concrete calculations, normalize the measure so that $\mathbb{C}P^{D-1}$'s total volume is unity, using:

$$\begin{aligned} d\mu_n &= \frac{dV_{FS}}{\mathrm{Vol}(\mathbb{C}P^n)} \\ &= \frac{n!}{(2\pi)^n} \prod_{k=1}^{n} dp_k \prod_{k=1}^{n} d\nu_k \ . \end{aligned}$$

This does not alter results in the main text. On the one hand, calculations of measurable quantities are independent of this value. On the other, here, at the calculation's end, we reintroduce the appropriate normalization.

We can now compute $W(\mathcal{E})$ for a generic quantum system. Assuming that $\delta\mathcal{E} \ll |E_{\max} - E_{\min}|$, we have $W(\mathcal{E}) = \Omega(\mathcal{E})\delta\mathcal{E}$ and $\Omega(\mathcal{E})$ is the area of the surface Σ defined by $h(Z) = \mathcal{E}$:

$$\Omega(\mathcal{E}) = \int_{\Sigma} d\sigma \ ,$$

where $d\sigma$ is the area element resulting from projecting both the symplectic two-form and the metric tensor onto the surface Σ. To compute this we choose an appropriate coordinate system:

$$\begin{aligned} Z^\alpha &= \langle E_\alpha | \psi(Z) \rangle \\ &= n_\alpha e^{i\nu_\alpha} \end{aligned}$$

adapted to the surface Σ:

$$\begin{aligned} h(Z) &= \langle \psi(Z) | \, H \, | \psi(Z) \rangle \\ &= \sum_{k=0}^{n} E_k | \langle \psi | E_k \rangle |^2 \\ &= \sum_{k=0}^{n} E_k n_k^2 \\ &= \mathcal{E} \ . \end{aligned}$$

On both sides we subtract the ground state energy E_0 and divide by $E_{\max} - E_0$ to obtain the following defining equation for $\Sigma \subset \mathbb{C}P^n$:

$$\begin{aligned} F(n_0, n_1, \ldots, n_n, \nu_1, \ldots, \nu_n) &= \sum_{k=0}^{n} \varepsilon_k n_k^2 - \varepsilon \\ &= 0 \ , \end{aligned}$$

with:

$$\begin{aligned} \varepsilon_k &= \frac{E_k - E_0}{E_{\max} - E_0} \in [0,1] \text{ and} \\ \varepsilon &= \frac{\mathcal{E} - E_0}{E_{\max} - E_0} \in [0,1] \ . \end{aligned}$$

We use octant coordinates for $\mathbb{C}P^n$:

$$(Z_0, Z_1, \ldots, Z_n) = \left(n_0, n_1 e^{i\nu_1}, n_2 e^{i\nu_2} \ldots, n_n e^{i\nu_n} \right) \ ,$$

where $n_k \in [0,1]$ and $\nu_k \in [0, 2\pi[$. With the transformation $p_k = n_k^2$ the equation for Σ becomes:

$$\sum_{k=0}^{n} p_k \varepsilon_k - \varepsilon = 0 \ .$$

a. Qubit Case

The state space of a single qubit is $\mathbb{C}P^1$. The latter's parametrization:

$$p\varepsilon_0 + (1-p)\varepsilon_1 = 1 - p$$

means that $h(Z) \leq \mathcal{E}$ is equivalent to $1 - p \leq \varepsilon$. The volume is therefore given by:

$$\begin{aligned} \mathrm{Vol}_{n=1}(\mathcal{E}) &= \frac{1}{\pi} \int_{h(\phi)\leq\mathcal{E}} dV_{FS} \\ &= \frac{1}{2\pi} \int_{1-\varepsilon}^{1} dp \int_{0}^{2\pi} d\nu \\ &= \varepsilon \\ &= \frac{\mathcal{E} - E_0}{E_1 - E_0} \ . \end{aligned}$$

In turn, this gives;

$$\begin{aligned} W_{n=1}(\mathcal{E}) &= \mathrm{Vol}_{n=1}(\mathcal{E}+\delta\mathcal{E}) - \mathrm{Vol}_{n=1}(\mathcal{E}) \\ &= \frac{1}{E_1 - E_0}\delta\mathcal{E} \ . \end{aligned}$$

In other words:

$$\Omega_{n=1}(\mathcal{E}) = \frac{1}{E_1 - E_0} \ ,$$

which is a constant density of states.

b. Qutrit Case

The state space of qutrits is $\mathbb{C}P^2$, with parametrization $Z = (Z_0, Z_1, Z_2) = (1-p-q, pe^{i\nu_1}, qe^{i\nu_2})$. With these coordinates, the equations defining the constant-energy hypersurface is:

$$(1-p-q)\varepsilon_0 + p\varepsilon_1 + q\varepsilon_2 = p\varepsilon_1 + q \leq \varepsilon \ .$$

And, it has volume:

$$\begin{aligned} \mathrm{Vol}_{n=2}(\mathcal{E}) &= \frac{2}{(2\pi)^2} \iint dqdq \iint d\nu_1 d\nu_2 \\ &= 2 \iint_S dpdq \ . \end{aligned}$$

In this, we have the surface $S := \left\{(p,q) \in \mathbb{R}^2 \ : p,q \geq 0, p+q \leq 1, q \leq \varepsilon - p\varepsilon_1\right\}$. Examining the geometry we directly see that the region's area is:

$$A(S) = \begin{cases} \frac{1}{2} - \frac{1}{2}\frac{(1-\varepsilon)^2}{1-\varepsilon_1} & \text{when } \varepsilon \geq \varepsilon_1 \\ \frac{\varepsilon^2}{2\varepsilon_1} & \text{when } \varepsilon < \varepsilon_1 \end{cases} \ .$$

Or:

$$A(S) = \begin{cases} \frac{1}{2} - \frac{1}{2}\frac{(E_2-\mathcal{E})^2}{(E_2-E_1)(E_2-E_0)} & \text{when } \mathcal{E} \geq E_1 \\ \frac{1}{2}\frac{(\mathcal{E}-E_0)^2}{(E_1-E_0)(E_2-E_0)} & \text{when } \mathcal{E} < E_1 \end{cases} \ .$$

One can check that the function $A(S)[\mathcal{E}]$ and its first derivative are continuous. Eventually, we have:

$$\begin{aligned} W_{n=2}(\mathcal{E}) &= \mathrm{Vol}_{n=2}(\mathcal{E}+\delta\mathcal{E}) - \mathrm{Vol}_{n=2}(\mathcal{E}) \\ &= \begin{cases} \frac{2(E_2-\mathcal{E})}{(E_2-E_1)(E_2-E_0)}\delta\mathcal{E} & \text{when } \mathcal{E} \geq E_1 \\ \frac{2(\mathcal{E}-E_0)}{(E_2-E_0)(E_1-E_0)}\delta\mathcal{E} & \text{when } \mathcal{E} < E_1 \end{cases} \ . \end{aligned}$$

c. Generic Qudit Case: $\mathbb{C}P^n$

To use Ref. [31]'s result, summarized in App. A, we must change coordinates. Again, using "probability + phase" coordinates:

$$\sum_{k=0}^{n} p_k E_k = \mathcal{E}$$

means that:

$$\begin{aligned} \sum_{k=1}^{n} p_k a_k &= t(\mathcal{E}) \\ a_k &= a(E_k) \\ &= \frac{E_k - E_0}{R} \ , \\ R &= \sqrt{\sum_{k=1}^{n} (E_k - E_0)^2}, \text{ and} \\ t(\mathcal{E}) &= \frac{\mathcal{E} - E_0}{R} \ . \end{aligned}$$

In this way, we can apply the result, finding:

$$\begin{aligned} \mathrm{Vol}_n\,(\mathcal{E}) &= \sum_{k=0}^{n} \frac{(t-a_k)_+^n}{\prod_{j\neq k\,,\,j=0}^{n}(a_j - a_k)} \\ &= \sum_{k=0}^{n} \frac{(\mathcal{E}-E_k)_+^n}{\prod_{j\neq k, j=0}^{n}(E_j - E_k)} \ . \end{aligned}$$

Since $\mathcal{E} \in [E_0, E_{\max}]$, there exists an $\overline{n}$ such that $\mathcal{E} \in]E_{\overline{n}}, E_{\overline{n}+1}[$. This means that the sum in the second term stops at $k = \overline{n}$ because after that $(\mathcal{E} - E_k)_+ = 0$. Hence, there exists $\overline{n}(\mathcal{E})$ such that for all $k > \overline{n}$ we have $(\mathcal{E} - E_k)_+ = 0$. This, in turns, shows that:

$$\mathrm{Vol}_n\,(\mathcal{E}) = \sum_{k=0}^{\overline{n}(\mathcal{E})} \frac{(\mathcal{E}-E_k)^n}{\prod_{j\neq k, j=0}^{n}(E_j - E_k)} \ .$$

This leads to the desired fraction of $\mathbb{C}P^n$ microstates in a microcanonical energy shell $[\mathcal{E}, \mathcal{E}+d\mathcal{E}]$:

$$\begin{aligned} W_n(\mathcal{E}) &= \Omega_n(\mathcal{E})d\mathcal{E} \\ &= \left(\sum_{k=0}^{\overline{n}(\mathcal{E})} \frac{n(\mathcal{E}-E_k)^{n-1}}{\prod_{j\neq k, j=0}^{n}(E_j - E_k)}\right) d\mathcal{E} \ . \end{aligned}$$

This allows defining the *statistical entropy* $S(\mathcal{E})$ of a quantum system with finite-dimensional Hilbert space of dimension $D = n+1$ as:

$$S(\mathcal{E}) = \log W_{D-1}(\mathcal{E}) \ .$$

3. Statistical physics of quantum states: Canonical ensemble

The continuous canonical ensemble is defined as:

$$\rho_\beta(\psi) = \frac{e^{-\beta h(\psi)}}{Q_\beta[h]} \ ,$$

where:

$$Q_\beta[h] = \int_{\mathbb{C}P^{D-1}} e^{-\beta h(\psi)} dV_{FS} \ .$$

The following analyzes the simple qubit case and then moves to the general treatment of a finite-dimensional Hilbert space $\mathcal{H}$.

a. Single Qubit

The Hilbert space here is $\mathcal{H}$ while the pure-state manifold is $\mathbb{C}P^1$. And so, we have:

$$Q_\beta[h] = \frac{1}{4}\int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi \ e^{-\beta h(\theta,\phi)} \ ,$$

with $h(\theta,\phi) = \vec{\gamma}\cdot\langle\vec{\sigma}\rangle = \vec{\gamma}\cdot\vec{b}(\theta,\phi)$.

Since we consider a single qubit, whose state space is S^2 embedded in $\mathbb{R}^3$, we can write $\vec{\gamma}\cdot\vec{b}(\psi) = \|\vec{\gamma}\|\cos\theta$, where θ is the angle between $\vec{\gamma}$ and $\vec{b}(\psi)$. Thus, we can use an appropriate coordinate $h(\phi,\theta) = \|\vec{\gamma}\|\cos\theta$ aligned with $\vec{\gamma}$ to find:

$$Q_\beta[h] = \pi\frac{\sinh\beta\|\vec{\gamma}\|}{\beta\|\vec{\gamma}\|} \ .$$

Or, using "probability + phase" coordinates (p,ν) we can also write:

$$\frac{1}{2}\int_0^1 dp \int_0^{2\pi} d\nu \ e^{-\beta[(1-p)E_0+pE_1]} = \pi\frac{e^{-\beta E_0}-e^{-\beta E_1}}{\beta(E_1-E_0)} \ .$$

The change in coordinates is given by the result of diagonalization: $E_0 = -\|\vec{\gamma}\|$ and $E_1 = \|\vec{\gamma}\|$. This yields the expected result:

$$\begin{aligned} Q_\beta[h] &= \pi\frac{e^{-\beta E_0}-e^{-\beta E_1}}{\beta(E_1-E_0)} \\ &= \pi\frac{\sinh\beta\|\vec{\gamma}\|}{\beta\|\vec{\gamma}\|} \ . \end{aligned}$$

b. Generic Treatment of $\mathbb{C}P^n$

We are now ready to address the general case of qudits:

$$\begin{aligned} Q_\beta[h] &= \int_{\mathbb{C}P^n} e^{-\beta h(Z)} dV_{FS} \\ &= \frac{1}{2^n}\int \prod_{k=0}^n e^{-\beta p_k E_k} \prod_{k=1}^n dp_k d\nu_k \\ &= \pi^n \int_{\Delta_n} \prod_{k=0}^n e^{-\beta p_k E_k} \delta\left(\sum_{k=0}^n p_k - 1\right) dp_1 \ldots dp_n \ . \end{aligned}$$

To evaluate the integral we first take the Laplace transform:

$$I_n(r) \coloneqq \int_{\Delta_n} \prod_{k=0}^n e^{-\beta p_k E_k} \delta\left(\sum_{k=0}^n p_k - r\right) dp_1 \ldots dp_n$$

to get:

$$\tilde{I}_n(z) \coloneqq \int_0^\infty e^{-zr} I(r) dr \ .$$

Calculating, we find:

$$\begin{aligned} \tilde{I}_n(z) &= \prod_{k=0}^n \frac{(-1)^k}{(\beta E_k + z)} \\ &= (-1)^{\frac{n(n+1)}{2}} \prod_{k=0}^n \frac{1}{z-z_k} \ . \end{aligned}$$

with $z_k = -\beta E_k \in \mathbb{R}$.

The function $\tilde{I}_n(z)$ has $n+1$ real and distinct poles: $z = z_k = -\beta E_k$. Hence, we can exploit the partial fraction decomposition of $\tilde{I}_n(z)$, which is:

$$(-1)^{\frac{n(n+1)}{2}} \prod_{k=0}^n \frac{1}{z-z_k} = (-1)^{\frac{n(n+1)}{2}} \sum_{k=0}^n \frac{R_k}{z-z_k} \ ,$$

where:

$$\begin{aligned} R_k &= \left[(z-z_k)\tilde{I}_n(z)\right]_{z=z_k} \\ &= \prod_{j=0,\, j\neq k}^n \frac{(-1)^{\frac{n(n+1)}{2}}}{z_k - z_j} \ . \end{aligned}$$

The inverse Laplace transform's linearity, coupled with the basic result:

$$\mathcal{L}^{-1}\left[\frac{1}{s+a}\right](t) = e^{-at}\Theta(t) \ ,$$

where:

$$\Theta(t) = \begin{cases} 1 & t \geq 0 \\ 0 & t < 0 \end{cases} \ ,$$

gives:

$$\begin{aligned} I_n(r) &= \mathcal{L}^{-1}[\tilde{I}_n(z)](r) \\ &= \Theta(r) \sum_{k=0}^{n} R_k e^{z_k r} \ . \end{aligned}$$

And so, we finally see that:

$$\begin{aligned} Q_\beta[h] &= I_n(1) \\ &= \sum_{k=0}^{n} \frac{e^{-\beta E_k}}{\prod_{j=0,\ j\neq k}^{n} (\beta E_k - \beta E_j)} \ . \end{aligned}$$

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