

UC Davis

UC Davis Previously Published Works

Title

Geometric Quantum Thermodynamics

Permalink

<https://escholarship.org/uc/item/6mm2q9h9>

Authors

Anza, Fabio
Crutchfield, James P

Publication Date

2020-08-19

Peer reviewed

Geometric Quantum Thermodynamics

Fabio Anza^{*} and James P. Crutchfield[†]

*Complexity Sciences Center and Physics Department,
University of California at Davis, One Shields Avenue, Davis, CA 95616*

(Dated: August 21, 2020)

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 develop both microcanonical and canonical ensembles, introducing continuous mixed states as distributions on the manifold of quantum states. We call out the experimental consequences for a gas of qudits. We define quantum heat and work in an intrinsic way, including single-trajectory work, and 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 Jarzynski's Fluctuation Theorem. The result is a more transparent physics, than conventionally available, in which the mathematical structure and physical intuitions underlying classical and quantum dynamics are seen to be closely aligned.

PACS numbers: 05.45.-a 89.75.Kd 89.70.+c 05.45.Tp

Keywords: quantum thermodynamics, differential geometry, classical thermodynamics, statistical mechanics

I. INTRODUCTION

The standard formulation of quantum mechanics defines a quantum system's (pure) states as normalized vectors $|\psi\rangle$ in a complex Hilbert space $\mathcal{H}$. There are alternative starting points, though. One is provided by the geometric formalism that describes states as points on a manifold. For finite-dimensional quantum systems—the ones we focus on here—the manifolds are complex projective spaces $\mathbb{CP}^n$ of dimension $n = D - 1$, where $D := \dim \mathcal{H}$. Our goal is to highlight the geometric approach's advantages when describing quantum dynamics and quantum thermodynamics. In particular, structural and informational properties can be properly formulated, since close parallels in the mathematical foundations of classical and quantum dynamics become clear.

This builds on two companion works. The first argues that geometric quantum states, not density matrices, completely characterize the state of quantum systems [1]. While the second connects to experiments, introducing a method to estimate them, via a maximum entropy principle, starting from knowledge of the density matrix [2].

To the best of our knowledge, such geometric formalisms started with early insights from Strocchi [3] and then work by Kibble [4], Heslot [5], Gibbons [6], Ashtekar and Shilling [7, 8], and a host of others [9–18]. 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 [22]. This arises, most directly, since the geometric formulation puts quantum mechanics on the same footing as the classical mechanics of phase space [3, 5], bringing to light the symplectic character of the geometry of the space of quantum states. 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.

However, this poses the conundrum of a consistent foundation of thermodynamic behavior. On the one hand, we have quantum statistical mechanics—a description of the macroscopic behavior which, despite its limitations, has proven to be remarkably successful. On the other hand, 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 appears as a challenging topic deserving of further attention. To address this, the following advocates a geometric development of a practical, macroscopic companion of geometric quantum statistical mechanics—a geometric quantum thermodynamics.

Geometric quantum thermodynamics is all the more timely due to recent success in driving thermodynamics down to the mesoscopic scale, where 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-clean crossover between them.

^{*} fanza@ucdavis.edu

[†] chaos@ucdavis.edu

The development unfolds as follows. First, we introduce the basic elements of geometric quantum mechanics. Second, we show how this formalism emerges naturally in a thermodynamic context. Third, we describe our version of the statistical treatment of geometric quantum mechanics—what we refer to as geometric quantum statistical mechanics. Fourth, we propose an experimental scenario that directly assesses its validity. Fifth, we build 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. Finally, we expand on the approach’s relevance and recommend future directions.

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 [3–18]. Here, we present the main ideas in a constructive way that builds on quantum mechanics’ familiar vector-based formalism.

Any statistical mechanics requires an appropriate, workable concept of ensemble. Here, this must be built out of geometric quantum states. We do this, identifying ensembles with coordinate-invariant measures on the manifold of pure states—what we call the continuous mixed states. Reaching 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 manifold of its pure states is a *complex projective space* $\mathcal{P}(\mathcal{H}) = \mathbb{C}P^{D-1}$ [10]. Given an arbitrary basis $\{|e_\alpha\rangle\}_{\alpha=0}^{D-1}$ a pure state is therefore 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 of a single qubit can be given by $Z_{\text{qubit}} = (\sqrt{p_0}, \sqrt{p_1}e^{i\nu})$. An observable $\mathcal{O}$ is a quadratic 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:

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

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

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

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

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

$$\Omega = 2ig_{\alpha\beta} dZ^\alpha \wedge d\bar{Z}^\beta ,$$

using shorthand $\bar{\partial}_\alpha := \partial/\partial\bar{Z}^\alpha$. It is not too hard to see that these two structures are parts of the Hermitian form which defines the scalar product $\langle\psi_1|\psi_2\rangle$ in Hilbert space. Indeed, using the form notation, one has [6]:

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

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 [10], based on the Fubini-Study metric on $\mathbb{C}P^{D-1}$:

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

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

Equipped with this unique volume, the total volume of the pure-state manifold is [6, 10]:

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

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 [3] and made particularly clear by Heslot [5]. Indeed, as in classical mechanics, the symplectic two-form 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:

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

where we used $\Omega = \frac{1}{2} \Omega_{\alpha\beta} dZ^\alpha \wedge d\bar{Z}^\beta$ and $\Omega^{\alpha\beta} = (\Omega^{-1})_{\alpha\beta}$

is the inverse: $\Omega^{\alpha\gamma}\Omega_{\gamma\beta} = \delta_{\beta}^{\alpha}$. 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:

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

$$\frac{dF}{dt} = \{F, h\} \quad (3b)$$

where $h(Z) = \sum_{\alpha\beta} H_{\alpha\beta} Z^{\alpha} \bar{Z}^{\beta}$ and $F : \mathcal{P}(\mathcal{H}) \rightarrow \mathbb{R}$ is a real but otherwise arbitrary function. Indeed, it can be shown that Schrödinger's equation is nothing but Hamilton's equations of motion in disguise [5, 10]:

$$\frac{d|\psi_t\rangle}{dt} = -iH|\psi_t\rangle \iff \frac{dF}{dt} = \{F, h\} , \quad (4)$$

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 [27]. 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 $|\psi\rangle \in \mathcal{H}$ 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: $\delta \rightarrow \delta/\det J$.

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:

$$P_{\psi_0}[\mathcal{O}] = \int_{\mathcal{P}(\mathcal{H})} \tilde{\delta}[Z - Z_0] \mathcal{O}(Z) dV_{FS} \quad (5)$$

$$\begin{aligned} &= \mathcal{O}(Z_0) \\ &= \langle \psi_0 | \mathcal{O} | \psi_0 \rangle , \end{aligned} \quad (6)$$

where:

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

and:

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

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

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

It is now quite natural to consider generalized ensembles that correspond to functionals with a continuous measure on the pure-state manifold. While such ensembles have appeared sporadically [9, 19–21], to the best of our knowledge an appropriate definition—one in which the distribution is invariant under coordinate changes—has not been given explicitly. We do this now.

Consider all series $S_N := \{p_k\}_{k=1}^N$ of normalized— $\sum_{k=1}^N p_k = 1$ —but otherwise arbitrary probability distributions that converge: $\lim_{N \rightarrow \infty} S_N = S$. Call $P_N[\mathcal{O}]$ the *pure-state functional* associated to S_N :

$$P_N[\mathcal{O}] = \sum_{k=1}^N p_k \int_{\mathcal{P}(\mathcal{H})} \tilde{\delta}[Z - Z_k] \mathcal{O}(Z) dV_{FS} . \quad (7)$$

We define the *geometric quantum state* as the limit $P_{\infty}[\mathcal{O}] := \lim_{N \rightarrow \infty} P_N[\mathcal{O}]$ of the pure-state functional:

$$P_{\infty}[\mathcal{O}] = \int_{\mathcal{P}(\mathcal{H})} p(Z) \mathcal{O}(Z) dV_{FS} , \quad (8)$$

with:

$$p(Z) = \lim_{N \rightarrow \infty} \sum_{k=1}^N p_k \frac{\delta[Z - Z_k]}{\sqrt{g}} .$$

The resulting continuous mixed 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 is also invariant under unitary transformations, thanks to the properties of the Fubini-Study volume element.

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 $|\psi_{AB}\rangle = \sum_{\alpha,i} \psi_{AB}^{\alpha i} |a_\alpha\rangle |b_i\rangle \in \mathcal{H}_{AB}$, the partial trace over the subsystem B is:

$$\rho^A = \sum_{\alpha,\beta=1}^{d_A} \rho_{\alpha\beta}^A |a_\alpha\rangle\langle a_\beta| ,$$

where:

$$\begin{aligned} \rho_{\alpha\beta}^A &= \sum_{i=1}^{d_B} \psi_{AB}^{\alpha i} \bar{\psi}_{AB}^{\beta i} \\ &= (\psi \psi^\dagger)_{\alpha\beta} . \end{aligned}$$

Hence, we can write this as:

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

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

$$|v_i\rangle := \sum_{\alpha=1}^{d_A} \psi_{AB}^{\alpha i} |a_\alpha\rangle .$$

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

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

This gives:

$$\begin{aligned} p_k^B &= \rho_{kk}^B \\ &= \sum_{\alpha=1}^{d_A} |\psi_{AB}^{\alpha k}|^2 . \end{aligned}$$

We see that $\langle v_j | v_k \rangle$ is a Gramian matrix of vectors $|v_j\rangle \in \mathcal{H}_A$ that conveys information on the marginalized components $\mathcal{H}_B$ into the reduced density matrix ρ^A . Though the vectors $|v_k\rangle$ are not normalized, we readily define their normalized counterpart:

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

And, eventually, we obtain:

$$\rho^A = \sum_{k=1}^{d_B} p_k^A |\chi_k^A\rangle\langle \chi_k^A| , \quad (9)$$

where:

$$\langle \chi_j | \chi_k \rangle = \sum_{\alpha=1}^{d_A} \frac{\psi_{AB}^{\alpha k} \bar{\psi}_{AB}^{\alpha j}}{\sqrt{p_k^B p_j^B}} .$$

and $\langle \chi_k | \chi_k \rangle = 1$.

This allows us to operationally define ρ_∞^A as the thermodynamic limit of ρ^A , for $d_B \rightarrow \infty$. The limit is done at fixed A and, as usual, keeps the energy density $\langle H \rangle / N$ finite, where H is the Hamiltonian of the entire system AB . The thermodynamic limit, though, raises new concerns.

While it is possible to track all information about $\{p_k^A\}_{k=1}^{d_B}$ 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 $\rho^A = \sum_{i=1}^{d_A} \lambda_i |\lambda_i\rangle\langle \lambda_i|$, where the λ_i are the Schmidt coefficients of $|\psi_{AB}\rangle$, is always available. However, this retains only ρ^A 's matrix elements, erasing the information contained in the vectors $|v_j\rangle = \sqrt{p_j^A} |\chi_j^A\rangle$.

That is, ρ^B has been erased from the description. However, this information can be crucial to understand the behavior of the small system A . The geometric formalism resolves this issue as it naturally keeps the information. It handles measures and probability distributions and, in the limit of the larger “environment” B , it allows working with an open system while retaining the information about its “purifying environment”.

To appreciate how this works, consider A 's geometric quantum state at fixed d_B :

$$p_{\rho^A}^{d_B}(\Gamma) := \sum_{k=1}^{d_B} p_k^B \tilde{\delta}[\Gamma - \chi_k] .$$

We can thus define its thermodynamic limit as:

$$\begin{aligned} P_{\rho^A}^\infty[O_A] &= \lim_{d_B \rightarrow \infty} P_{\rho^A}[O_A] \\ &= \int_{\mathcal{P}_A} dV_{FS}^A O_A(\Gamma) p_{\rho^A}^\infty(\Gamma) , \end{aligned}$$

with:

$$p_{\rho^A}^\infty(\Gamma) := \lim_{d_B \rightarrow \infty} \sum_{k=1}^{d_B} p_k^B \tilde{\delta}[\Gamma - \chi_k] .$$

P^∞ is the continuous counterpart of a standard density matrix and its operational meaning is understood in terms of ensemble theory, mirroring the way in which we interpret the discrete probability distribution $\{p_k\}$ for a standard density matrix $\rho = \sum_k p_k |\psi_k\rangle\langle \psi_k|$. Discrete and continuous mixed states describe ensembles of independent and noninteracting instances of the same quantum system whose pure states are distributed according to a given probability distribution. In other words, if we pick a random pure state out of the ensemble described

by P^∞ , the probability of finding it in a small region of size dV_{FS} around Z is $dP_Z = p(Z)dV_{FS}$.

The following 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. Assuming repeatability, we perform tomography and sequentially record the states as points on $\mathbb{CP}^1$. Their distribution is generically denoted $p(\theta, \phi)$. 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 obey a canonical distribution $\gamma_\beta = e^{-\beta H}/Z_\beta$.

However, one immediately sees that the standard treatment of quantum statistical mechanics contains an unwanted assumption. After we extract the k -th sample from the macroscopic system, that sample's state is supposed to be an energy eigenstate $|E_i^{(k)}\rangle$ with probability $p(Z(|E_i^{(k)}\rangle)) \propto e^{-\beta E_i^{(k)}}$. There is, however, no reason to assume that the Hamiltonians H_k of all the samples are identical to each other. In fact, $|E_i^h\rangle \neq |E_i^k\rangle$ and $E_i^h \neq E_i^k$.

To address this, we posit that a more appropriate description of the system's state is given by the continuous counterpart of Gibbs canonical state, written as the following functional:

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

where:

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

with $h(Z) = \sum_{\alpha\beta} H_{\alpha\beta} Z^\beta \bar{Z}^\alpha$. While this distribution retains a characteristic feature of the canonical Gibbs ensemble— $p(Z(|E_n\rangle))/p(Z(|E_m\rangle)) = e^{-\beta(E_n - E_m)}$ —it also extends this “Boltzmann” rule to arbitrary states:

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

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:

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

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 introducing an alternative formulation of the statistical mechanics of quantum systems—one based on continuous mixed states rather than on the familiar discrete states.

IV. STATISTICAL TREATMENT OF GEOMETRIC QUANTUM MECHANICS

Representing the state of a quantum system 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 these 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 the phase space of an isolated system, *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 probability distribution P_{mc} of finding the system in a microstate $(\vec{p}, \vec{q})$ is, at equilibrium:

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

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

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

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 $E_n \in I_{\text{mc}}$:

$$p_{\text{mc}}(E_n) = \begin{cases} W_{\text{mc}} & \text{if } E_n \in [\mathcal{E}, \mathcal{E} + \delta\mathcal{E}] \\ 0 & \text{otherwise} \end{cases}.$$

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 now introduce.

C. Geometric quantum microcanonical ensemble: A priori equal probability

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

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

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 the Liouville dynamics on the manifold of the pure states $\mathcal{P}(\mathcal{H})$, it is easy to see that there is a straightforward geometric implementation of the a-priori-equal-probability postulate in the quantum setting:

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

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

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

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 [5] 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 $[X] = [\sqrt{\hbar}] = \text{Length}\sqrt{\text{Mass}/\text{Time}}$ and $[Y] = [\sqrt{\hbar}] = \text{Momentum}\sqrt{\text{Time}/\text{Mass}}$. 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:

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

where 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 from that of $\mathcal{P}(\mathcal{H})$ due to the constraints $\sum_{k=1}^{D-1} (X^k + Y^k)^2 \leq 1$ and $X^k, Y^k \geq 0$.

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

$$\omega(\mathcal{E}) = \frac{\pi^{D-1}}{(D-1)!} \sum_{k=0}^{\bar{n}(\mathcal{E})} \frac{(D-1)(\mathcal{E} - E_k)^{D-2}}{\prod_{j \neq k, j=0}^{D-1} (E_j - E_k)}. \quad (10)$$

This is in agreement with Ref. [20]'s Eq. (5), which was given without proof. Here we fill this gap and, in Appendix II C, provide a detailed proof, using a convenient mathematical result by Lasserre [28].

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:

$$p_\beta(Z) = \frac{e^{-\beta h(Z)}}{Q_\beta[\hbar]}, \quad (11)$$

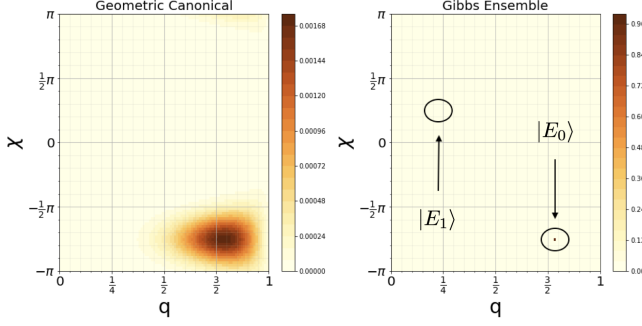


Figure 1. Alternate ensembles in the standard and geometric settings: Differences are plainly evident. Canonical probability distributions on a qubit's state manifold $\mathbb{CP}^1$ with coordinates $Z = (Z^0, Z^1) = (\sqrt{1-q}, \sqrt{q}e^{i\chi})$ where $q \in [0, 1]$ and $\chi \in [-\pi, \pi]$. $\mathbb{CP}^1$ 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 $dV_{FS} = dq d\chi/2$. The Hamiltonian is $H = \sigma_x + \sigma_y + \sigma_z$, with $\hbar = 1$ and inverse temperature $\beta = 5$ ($k_B = 1$). (Right) Gibbs ensemble where circles enclose the positions around the coordinates of the respective eigenvectors $(q(|E_0\rangle), \chi(|E_0\rangle)) = (0.789, -2.356)$ and $(q(|E_1\rangle), \chi(|E_1\rangle)) = (0.211, 0.785)$. (Left) Geometric Canonical Ensemble.

where:

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

Reference [19] first proposed the canonical partition function $Q_\beta[h]$ in specific low-dimensional cases. A follow-on work [20] gave a generic representation for arbitrary finite-dimensional Hilbert spaces, but without proof. Appendix II C, here, fills this gap, providing a proof and explicit examples of:

$$Q_\beta[h] = \sum_{k=0}^{D-1} \frac{e^{-\beta E_k}}{\prod_{j=0, j \neq k}^n (\beta E_k - \beta E_j)}. \quad (12)$$

This is in full agreement with Ref. [20]'s Eq. (6). Figure 1 plots the standard Gibbs ensemble (Right) and its geometric counterpart (Left) for the Hamiltonian $H = \sigma_x + \sigma_y + \sigma_z$ at inverse temperature $\beta = 5$.

With the ensembles laid out we can now highlight the geometric framework's experimental consequences. The next section presents a proposal to discriminate between standard and geometric ensembles.

V. EXPERIMENTAL RELEVANCE: QUDIT GAS

With its ensemble theory, the standard machinery of quantum statistical mechanics turns on a system being diagonal in the Hamiltonian basis. And, this means that

superpositions between different energy eigenstates are not allowed. While this is consistent with several experimental results, this cannot always be the case. We present an experimentally-concrete scenario that clearly violates this assumption, demonstrating the necessity of statistical geometric quantum mechanics.

Consider a box containing a gas of N weakly interacting quantum systems (qudits) with finite Hilbert space of dimension D . Let's treat the spatial degrees of freedom classically while applying a full quantum treatment to the internal degrees of freedom. Prepare the system in a product state $|\psi\rangle = \otimes_{k=1}^N |\psi_k\rangle$ and let it evolve unitarily with Hamiltonian $H = H_0 + H_I$, where $H_0 = \sum_{k=1}^N H_k$. Here, H_0 is the single-body Hamiltonian and H_I is a two-body interaction Hamiltonian. The interaction is weak in the sense that $\|H_I\|_F \ll \|H_0\|_F$, where we use the Frobenius matrix norm: $\|A\|_F := \sqrt{\sum_{i,j} |A_{ij}|^2}$. We also assume that H_I 's presence removes possible degeneracies present in H_0 so that H 's spectrum is nondegenerate.

To simplify the treatment, set $D = 2$. Let the box have a small hole from which qubits escape. The hole is connected to a Stern-Gerlach measurement apparatus that performs a von Neumann measurement $\{\Pi_{\pm}^{(\theta, \phi)}\}$ with:

$$\Pi_{+}^{(\theta, \phi)} := |\psi(\theta, \phi)\rangle \langle \psi(\theta, \phi)| \quad \text{and} \quad (13a)$$

$$\Pi_{-}^{(\theta, \phi)} := |\psi_{\perp}(\theta, \phi)\rangle \langle \psi_{\perp}(\theta, \phi)| \quad (13b)$$

where:

$$\begin{aligned} |\psi(\theta, \phi)\rangle &:= \cos \theta/2 |0\rangle + e^{i\phi} \sin \theta/2 |1\rangle \quad \text{and} \\ |\psi_{\perp}(\theta, \phi)\rangle &:= \sin \theta/2 |0\rangle + e^{i(\phi+\pi)} \cos \theta/2 |1\rangle. \end{aligned}$$

On the one hand, according to the general precepts of quantum statistical mechanics the outcome probabilities $p_{\pm}(\theta, \phi)$ should be, up to experimental uncertainties:

$$\begin{aligned} p_{\pm}^{\text{Gibbs}}(\theta, \phi) &= \frac{e^{-\beta E_0}}{Z_\beta} \langle E_0 | \Pi_{\pm}^{(\theta, \phi)} | E_0 \rangle + \\ &\quad + \frac{e^{-\beta E_1}}{Z_\beta} \langle E_1 | \Pi_{\pm}^{(\theta, \phi)} | E_1 \rangle \end{aligned}$$

On the other hand, statistical geometric quantum mechanics predicts a different answer:

$$p_{\pm}^{\text{Geo}}(\theta, \phi) = \frac{1}{Q_\beta[h]} \int_{\mathcal{P}(\mathcal{H})} e^{-\beta h(Z)} P_{\pm}^{(\theta, \phi)}(Z),$$

where

$$\begin{aligned} P_{+}^{\theta, \phi}(Z) &= \langle \psi(Z) | \Pi_{+}^{(\theta, \phi)} | \psi(Z) \rangle \\ &= (\cos \theta/2)^2 |Z^0|^2 + (\sin \theta/2)^2 |Z^1|^2 \\ &\quad + \sin \theta \frac{e^{i\phi} Z^0 \bar{Z}^1 + e^{-i\phi} \bar{Z}^0 Z^1}{2}, \end{aligned}$$

and:

$$P_-^{\theta,\phi}(Z) = 1 - P_+^{\theta,\phi}(Z) .$$

The experimental protocol generalizes directly to a Hilbert space of arbitrary dimension D . As concrete example, fixing the von Neumann measure to lie along the z axis, Fig. 2 compares the temperature-dependent behavior of σ_z 's thermal average and standard deviation according to the Gibbs ensemble versus its geometric canonical counterpart. The system Hamiltonian is chosen to be the same as before: $H = \sigma_x + \sigma_y + \sigma_z$. This symmetry guarantees that the results associated with projective measurements of σ_x , σ_y , and σ_z are the same.

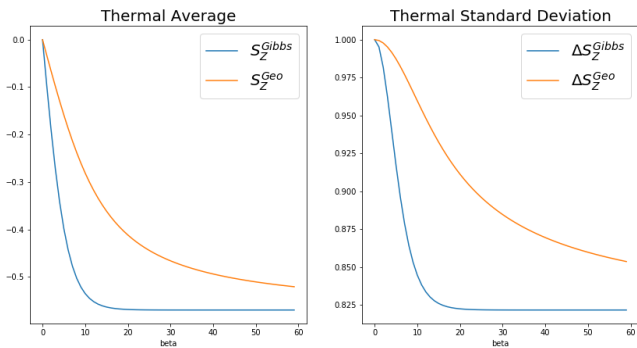


Figure 2. Gibbs and geometric canonical ensemble comparison: β -dependent behavior of the average (lefthand side) and standard deviation (righthand side) of a projective measurement along the z axis. While the qualitative dependence on β for the Gibbs ensemble and the geometric canonical ensemble appears similar, quantitative differences are clear, both for the average (S_z^{Gibbs} versus S_z^{Geo}) and for the fluctuations ($\Delta S_z^{\text{Gibbs}}$ versus ΔS_z^{Geo}).

VI. GEOMETRIC QUANTUM THERMODYNAMICS

With a consistent statistical geometric quantum mechanics in hand, we can now reformulate the thermodynamics of quantum systems. The thermodynamics behavior is modeled via the geometric canonical state Eq.(11). Notice that, in this setting, an appropriate entropy definition has yet to be given. Paralleling early work by Gibbs, consider the functional:

$$H_q[p] = -k_B \int_{\mathcal{P}(\mathcal{H})} p(Z) \log p(Z) dV_{FS} .$$

A basic information-theoretic analysis of this functional was done in Ref. [29].

Let's consider its role, though, for the quantum foundations of thermodynamics. In particular, assuming that the probability distribution of quantum states is thermal, we explore if this functional can provide an actionable

alternative to the von Neumann one, for a thermodynamic entropy. For the geometric canonical ensemble of Eq. (11), this gives:

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

where:

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

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:

$$dU = \int_{\mathcal{P}(\mathcal{H})} dV_{FS} p(Z) (dh)(Z) + \int_{\mathcal{P}(\mathcal{H})} dV_{FS} (dp)(Z) h(Z) = dW + dQ , \quad (14)$$

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:

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

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

$$dU = T dH_q + dF ,$$

where $T := (k_B \beta)^{-1}$.

B. Second Law

The Second Law follows from the Crooks [30] and Jarzynski [31] fluctuation theorems [26, 32, 33]. 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:

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

One can now leverage Jarzynski’s original argument [34] for 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. (11) and is then driven with a Hamiltonian that depends on a parameter λ following the time-dependent protocol $\lambda = \lambda(t)$ with $t \in [0, 1]$. An ensemble of several protocol realizations is realized. And, we can define the *single-trajectory work* as:

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

where $Z(\psi_t)$ are the homogeneous coordinates on $\mathbb{CP}^{D-1}$ for $|\psi_t\rangle$ and, therefore, are the solutions of Eq. (4).

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

$$\begin{aligned} \langle e^{-\beta W} \rangle_{\text{ens}} &= \frac{Q_\beta[h(\lambda_f)]}{Q_\beta[h(\lambda_i)]} \\ &= e^{-\Delta F} , \end{aligned} \quad (15)$$

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:

$$\langle e^{-\beta W} \rangle_{\text{ens}} \geq e_{\text{ens}}^{-\beta \langle W \rangle}$$

to obtain the Second Law’s familiar form:

$$\langle W \rangle_{\text{ens}} \geq F . \quad (16)$$

VII. DISCUSSION

While standard quantum mechanics is firmly rooted in an algebraic formalism, a geometric alternative based on the differential geometry of the quantum-state manifold $\mathcal{P}(\mathcal{H}) = \mathbb{CP}^{D-1}$ is readily available.

As previous works repeatedly emphasized [3, 5, 10], the geometric approach brings quantum and classical mechanics much closer. In both cases the manifold of states is a Kähler space, with two intertwined notions of geometry—Riemannian and symplectic.

Moreover, the quantum-state manifold sports a preferred notion of measure, selected by invariance under unitary transformations—the Fubini-Study measure. We exploited it to define continuous probability distributions on the quantum-state manifold as the infinite limit of convex combinations of Dirac-delta distributions. The resulting formalism is equivalent to the standard one in familiar cases. However, it allows working with a new

kind of quantum state, dubbed the *geometric quantum state* [1], that generalizes the familiar density matrix and provides more information about a quantum system’s physical configuration.

Leveraging parallels between the geometric formalism and classical mechanics, we introduced an alternative development for the statistical physics of quantum systems. Built on the geometric approach to quantum mechanics, this led to a continuous counterpart of Gibbs ensembles, which we call *continuous mixed states*. The microcanonical and canonical continuous ensembles were then presented and specific forms for the respective partition functions were derived. Remarkably, predictions from standard quantum statistical mechanics and its geometric counterpart differ. This posed a challenge: Which theory should one use? To address this, Sec. V proposed a concrete experiment with which to directly probe, by means of simple projective measurements, the different predictions.

Rounding out the development, Sec. VI laid out how to establish quantum thermodynamics on the basis of the geometric formalism. Building on Sec. IV’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 existing ones, derived within standard quantum statistical mechanics, they involve quantities that are genuinely different. It is interesting to observe how the fundamental laws appear formalism-independent, yielding functional relations between quantities that must be mutually consistent. Understanding how Eqs. (14), (15), and (16) connect to their standard counterparts [26] is a challenge that we must leave for the future.

VIII. CONCLUSION

Let’s conclude by highlighting an important feature that, so far, we did not make explicit. The geometric formalism and the emergence of continuous mixed states, introduced in the prequel Ref. [1], suggest a new concept of Boltzmann entropy for quantum states—one markedly closer to that in classical statistical mechanics:

$$S_B^q := k_B \log W ,$$

where W is the volume of accessible microstates in the complex projective manifold $\mathbb{CP}^{D-1}$.

Along similar lines, we considered extending Shannon’s informational functional to a nonmicrocanonical continuous ensemble:

$$H_q[p] = -k_B \int_{\mathcal{P}(\mathcal{H})} p(Z) \log p(Z) dV_{FS} .$$

When the probability distribution over the manifold of the states is discrete (convex combinations of Dirac-deltas) this becomes formally equivalent to the von Neumann

entropy functional. Moreover, these two notions of thermodynamic entropy (S_B^q and H_q) are conceptually identical to their classical counterpart: They evaluate the volume of microstates compatible with certain macroscopic conditions. This is a major conceptual difference with the standard treatment of quantum statistical mechanics, which is founded on the concept of von Neumann entropy. However, from the perspective of dynamical systems theory—arguably the umbrella under which both classical and quantum mechanics live—there is no conceptual difference. We believe the new concept of entropy deserves further attention, for example, by connecting to experiment via the maximum entropy estimation of geometric quantum states [2].

ACKNOWLEDGMENTS

F.A. thanks Marina Radulaski, Davide Pastorello, and Davide Girolami for discussions on the geometric formalism of quantum mechanics. F.A. and J.P.C. thank David Gier, Dhruva Karkada, Samuel Loomis, and Ariadna Venegas-Li for helpful discussions and the Telluride Science Research Center for its hospitality during visits. This material is based upon work supported by, or in part by, a Templeton World Charity Foundation Power of Information Fellowship, FQXi Grant FQXi-RFP-IPW-1902, and U.S. Army Research Laboratory and the U. S. Army Research Office under contracts W911NF-13-1-0390 and W911NF-18-1-0028.

DATA AVAILABILITY STATEMENT

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

-
- [1] F. Anza and J. P. Crutchfield. Beyond density matrices: Geometric quantum states. *in preparation*, 2020. [1](#), [9](#)
 - [2] F. Anza and J. P. Crutchfield. Geometric quantum state estimation. *in preparation*, 2020. [1](#), [10](#)
 - [3] F. Strocchi. Complex Coordinates and Quantum Mechanics. *Rev. Mod. Physics*, 38(1):36–40, 1966. [1](#), [2](#), [9](#)
 - [4] T. W. B. Kibble. Geometrization of quantum mechanics. *Communications in Mathematical Physics*, 65(2):189–201, jun 1979. [1](#)
 - [5] A. Heslot. Quantum mechanics as a classical theory. *Phys. Rev. D*, 31(6):1341–1348, mar 1985. [1](#), [2](#), [3](#), [6](#), [9](#)
 - [6] G.W. Gibbons. Typical states and density matrices. *J. Geom. Physics*, 8(1-4):147–162, 1992. [1](#), [2](#)
 - [7] A. Ashtekar and T. A. Schilling. Geometry of quantum mechanics. In *AIP Conference Proceedings*, volume 342, pages 471–478. AIP, 1995. [1](#)
 - [8] A. Ashtekar and T. A. Schilling. Geometrical Formulation of Quantum Mechanics. In *On Einstein's Path*, pages 23–65. Springer New York, New York, NY, 1999. [1](#)
 - [9] D. C. Brody and L. P. Hughston. Geometric quantum mechanics. *J. Geom. Physics*, 38(1):19–53, 2001. [1](#), [3](#)
 - [10] I. Bengtsson and K. Życzkowski. *Geometry of Quantum States*. Cambridge University Press, Cambridge, 2017. [2](#), [3](#), [9](#)
 - [11] J. F. Cariñena, J. Clemente-Gallardo, and G. Marmo. Geometrization of quantum mechanics. *Theor. Math. Physics*, 152(1):894–903, 2007.
 - [12] D. Chruściński. Geometric Aspects of Quantum Mechanics and Quantum Entanglement. *J. Physics: Conf. Ser.*, 30:9–16, 2006.
 - [13] G. Marmo and G. F. Volkert. Geometrical description of quantum mechanics—transformations and dynamics. *Physica Scripta*, 82(3):038117, 2010.
 - [14] J. Avron and O. Kenneth. An elementary introduction to the geometry of quantum states with pictures. *Rev. Math. Physics*, 32(02):2030001, 2020.
 - [15] D. Pastorello. A geometric Hamiltonian description of composite quantum systems and quantum entanglement. *Intl. J. Geom. Meth. Mod. Physics*, 12(07):1550069, 2015.
 - [16] D. Pastorello. Geometric Hamiltonian formulation of quantum mechanics in complex projective spaces. *Intl. J. Geom. Meth. Mod. Physics*, 12(08):1560015, sep 2015.
 - [17] D. Pastorello. Geometric Hamiltonian quantum mechanics and applications. *Intl. J. Geom. Meth. Mod. Physics*, 13(Supp. 1):1630017, 2016.
 - [18] J. Clemente-Gallardo and G. Marmo. The Ehrenfest picture and the geometry of Quantum Mechanics. *Il Nuovo Cimento C*, 3:35–52, 2013. [1](#), [2](#)
 - [19] D. C. Brody and L. P. Hughston. The quantum canonical ensemble. *J. Math. Physics*, 39(12):6502–6508, 1998. [1](#), [3](#), [5](#), [7](#)
 - [20] D. C. Brody, D. W. Hook, and L. P. Hughston. On quantum microcanonical equilibrium. *J. Physics: Conf. Ser.*, 67:012025, 2007. [5](#), [6](#), [7](#)
 - [21] D. C. Brody and L. P. Hughston. Thermodynamics of quantum heat bath. *J. Physics A: Math. Theo.*, 49(42):425302, 2016. [1](#), [3](#)
 - [22] D. C. Brody, D. W. Hook, and L. P. Hughston. Quantum phase transitions without thermodynamic limits. *Proc. Roy. Soc. A: Math. Phys. Engin. Sci.*, 463(2084):2021–2030, 2007. [1](#)
 - [23] U. Seifert. Stochastic thermodynamics: Principles and perspectives. *Euro. Phys. J. B*, 64(3-4):423–431, 2008. [1](#)
 - [24] U. Seifert. Stochastic thermodynamics, fluctuation theorems and molecular machines. *Rep. Prog. Physics*, 75(12):126001, dec 2012. [1](#)
 - [25] J. Gemmer, M. Michel, and G. Mahler. *Quantum Thermodynamics*, volume 657 of *Lecture Notes in Physics*. Springer Berlin Heidelberg, Berlin, Heidelberg, 2004. [1](#)

- [26] S. Deffner and S. Campbell. *Quantum Thermodynamics*. IOP Publishing, 2019. [1](#), [8](#), [9](#)
- [27] F. Strocchi. *An introduction to the mathematical structure of quantum mechanics: A short course for mathematicians*. World Scientific, Singapore, 2008. [3](#)
- [28] J. B. Lasserre. Volume of slices and sections of the simplex in closed form. *Optimization Letters*, 9(7):1263–1269, 2015. [6](#), [1](#), [4](#)
- [29] D. C. Brody and L. P. Hughston. Information content for quantum states. *J. Math. Physics*, 41(5):2586–2592, 2000. [8](#)
- [30] G. E. Crooks. Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences. *Phys. Rev. E*, 60(3):2721–2726, 1999. [8](#)
- [31] C. Jarzynski. Equalities and Inequalities: Irreversibility and the Second Law of Thermodynamics at the Nanoscale. *Ann. Rev. Cond. Matt. Physics*, 2(1):329–351, 2011. [8](#)
- [32] M. Campisi, P. Hänggi, and P. Talkner. Colloquium: Quantum fluctuation relations: Foundations and applications. *Rev. Mod. Phys.*, 83(3):771–791, 2011. [8](#)
- [33] R. Klages, W. Just, and C. Jarzynski. *Nonequilibrium statistical physics of small systems: Fluctuation relations and beyond*. Wiley-VCH, 2013. [8](#)
- [34] C Jarzynski. Nonequilibrium Equality for Free Energy Differences. *Phys. Rev. Lett.*, 78(14):2690–2693, 1997. [9](#)

Supplementary Materials

Geometric Quantum Thermodynamics

Fabio Anza and James P. Crutchfield

The following presents proofs and detailed calculations supporting the main text's claims.

I. INDEPENDENT RESULT

For completeness, the following summarizes Ref. [28]'s result called on in calculating the density of states. Given the n -simplex $\Delta_n : \{\vec{x} \in \mathbb{R}_+^n : \vec{e} \cdot \vec{x} \leq 1\}$, 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:

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

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

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

and:

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

II. 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.

A. 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 $\mathbb{C}P^n$. A point on the manifold is a set of D homogeneous and complex coordinates Z^α . A point corresponds to a pure state with the identification $Z \leftrightarrow |\psi\rangle = \sum_{\alpha=0}^{D-1} Z^\alpha |e_\alpha\rangle$, where $\{|e_\alpha\rangle\}_\alpha$ 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:

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

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 $\mathbb{C}P^{D-1}$.

B. Microcanonical density of states: Proof of Eq. (10)

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

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

Due to normalization we have:

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

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

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

This gives the manifold volume:

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

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

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

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 $\delta E \ll |E_{\text{max}} - E_{\text{min}}|$, we have $W(\mathcal{E}) = \Omega(\mathcal{E})\delta E$ 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 $\Sigma \subset \mathbb{C}P^n$:

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

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 $\mathbb{C}P^n$:

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

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:

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

1. 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:

$$\begin{aligned}
\text{Vol}_{n=1}(\mathcal{E}) &= \frac{1}{\pi} \int_{h(\phi) \leq \mathcal{E}} dV_{FS} \\
&= \frac{1}{2\pi} \int_{1-\varepsilon}^1 dp \int_0^{2\pi} d\nu \\
&= \varepsilon \\
&= \frac{\mathcal{E} - E_0}{E_1 - E_0} .
\end{aligned}$$

In turn, this gives;

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

In other words:

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

which is a constant density of states.

2. Qutrit Case

The state space of qutrits is $\mathbb{CP}^2$, 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:

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

In this, we have the surface $S := \{(p, q) \in \mathbb{R}^2 : p, q \geq 0, p + q \leq 1, q \leq \varepsilon - p\varepsilon_1\}$. 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:

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

3. Generic Qudit Case: $\mathbb{CP}^n$

To use Ref.[28]'s result, summarized in App. I, 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:

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

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

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

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

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

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

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

C. 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 $\mathcal{H}$.

1. Single Qubit

The Hilbert space here is $\mathcal{H}$ while the pure-state manifold is $\mathbb{CP}^1$. 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 and 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:

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

2. Generic Treatment of $\mathbb{CP}^n$

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

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

To evaluate the integral we first Laplace transform:

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

to get:

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

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:

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