

UC Davis

UC Davis Previously Published Works

Title

Geometric quantum thermodynamics

Permalink

<https://escholarship.org/uc/item/1w91727x>

Journal

Physical Review E, 106(5)

ISSN

2470-0045

Authors

Anza, Fabio
Crutchfield, James P

Publication Date

2022-11-01

DOI

10.1103/physreve.106.054102

Copyright Information

This work is made available under the terms of a Creative Commons Attribution-NonCommercial-NoDerivatives License, available at <https://creativecommons.org/licenses/by-nc-nd/4.0/>

Peer reviewed

Important Notice to Authors

No further publication processing will occur until we receive your response to this proof.

Attached is a PDF proof of your forthcoming article in PRE. Your article has 15 pages and the Accession Code is **QX10041E**.

Please note that as part of the production process, APS converts all articles, regardless of their original source, into standardized XML that in turn is used to create the PDF and online versions of the article as well as to populate third-party systems such as Portico, Crossref, and Web of Science. We share our authors' high expectations for the fidelity of the conversion into XML and for the accuracy and appearance of the final, formatted PDF. This process works exceptionally well for the vast majority of articles; however, please check carefully all key elements of your PDF proof, particularly any equations or tables.

Figures submitted electronically as separate files containing color appear in color in the online journal. However, all figures will appear as grayscale images in the print journal unless the color figure charges have been paid in advance, in accordance with our policy for color in print (<https://journals.aps.org/authors/color-figures-print>).

Specific Questions and Comments to Address for This Paper

- 1 Please note change and see the following: <http://publish.aps.org/authors/new-novel-policy-physical-review>.
 - 2 The citation of Fig. 1 is missing in the text. Please cite the same in running text in sequence to avoid the renumbering of floating elements.
 - 3 Please note that Fig. 1 was not cited in text. Please cite as appropriate.
- FQ:** This funding provider could not be uniquely identified during our search of the FundRef registry (or no Contract or Grant number was detected). Please check information and amend if incomplete or incorrect.
- Q:** This reference could not be uniquely identified due to incomplete information or improper format. Please check all information and amend if applicable.

ORCIDs: Please follow any ORCID links (🔗) after the authors' names and verify that they point to the appropriate record for each author. Requests to add ORCIDs should be sent no later than the first proof revisions. If authors do not subsequently add/authenticate ORCIDs within seven business days, production of the paper will proceed and no further requests to add ORCIDs will be processed. See complete details regarding ORCID requests and ORCID verification at <https://journals.aps.org/authors/adding-orcids-during-proof-corrections>.

NOTE: If this paper is an Erratum or a Reply, the corresponding author's ORCID may be present if previously provided to APS, but no ORCIDs can be added at proof stage.

Crossref Funder Registry ID: Information about an article's funding sources is now submitted to Crossref to help you comply with current or future funding agency mandates. Crossref's Funder Registry (<https://www.crossref.org/services/funder-registry/>) is the definitive registry of funding agencies. Please ensure that your acknowledgments include all sources of funding for your article following any requirements of your funding sources. Where possible, please include grant and award ids. Please carefully check the following funder information we have already extracted from your article and ensure its accuracy and completeness:

Templeton World Charity Foundation (BS), FQXi-RFP-IPW-1902
U. S. Army Research Office (US), W911NF-18-1-0028, W911NF-21-1-0048

Other Items to Check

- Please note that the original manuscript has been converted to XML prior to the creation of the PDF proof, as described above. Please carefully check all key elements of the paper, particularly the equations and tabular data.
- Title: Please check; be mindful that the title may have been changed during the peer-review process.
- Author list: Please make sure all authors are presented, in the appropriate order, and that all names are spelled correctly.
- Please make sure you have inserted a byline footnote containing the email address for the corresponding author, if desired. Please note that this is not inserted automatically by this journal.
- Affiliations: Please check to be sure the institution names are spelled correctly and attributed to the appropriate author(s).
- Receipt date: Please confirm accuracy.
- Acknowledgments: Please be sure to appropriately acknowledge all funding sources.
- Hyphenation: Please note hyphens may have been inserted in word pairs that function as adjectives when they occur before a noun, as in "x-ray diffraction," "4-mm-long gas cell," and "R-matrix theory." However, hyphens are deleted from word pairs when they are not used as adjectives before nouns, as in "emission by x rays," "was 4 mm in length," and "the R matrix is tested."

Note also that Physical Review follows U.S. English guidelines in that hyphens are not used after prefixes or before suffixes: superresolution, quasiequilibrium, nanoprecipitates, resonancelike, clockwise.

- Please check that your figures are accurate and sized properly. Make sure all labeling is sufficiently legible. Figure quality in this proof is representative of the quality to be used in the online journal. To achieve manageable file size for online delivery, some compression and downsampling of figures may have occurred. Fine details may have become somewhat fuzzy, especially in color figures. The print journal uses files of higher resolution and therefore details may be sharper in print. Figures to be published in color online will appear in color on these proofs if viewed on a color monitor or printed on a color printer.
- Please check to ensure that reference titles are given as appropriate.
- Overall, please proofread the entire *formatted* article very carefully. The redlined PDF should be used as a guide to see changes that were made during copyediting. However, note that some changes to math and/or layout may not be indicated.

Ways to Respond

- **Web:** If you accessed this proof online, follow the instructions on the web page to submit corrections.
- **Email:** Send corrections to preproofs@aptaracorp.com
Subject: **QX10041E** proof corrections
- **Fax:** Return this proof with corrections to +1.703.791.1217. Write **Attention: PRE Project Manager** and the Article ID, **QX10041E**, on the proof copy unless it is already printed on your proof printout.

Geometric quantum thermodynamics

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

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



(Received 29 May 2022; accepted 3 October 2022; published xxxxxxxxx)

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 Jarzynski'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.

DOI: [10.1103/PhysRevE.00.004100](https://doi.org/10.1103/PhysRevE.00.004100)

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 $D := \dim \mathcal{H}$. 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 lay out 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. Second, it shows how this formalism emerges naturally in a thermodynamic context. Third, it describes our version of the statistical

^{*}fanza@ucdavis.edu

[†]chaos@ucdavis.edu

81 treatment of geometric quantum mechanics, what we refer to
 82 as geometric quantum statistical mechanics. Fourth, it builds
 83 on this to establish two fundamental equations of geomet-
 84 ric quantum thermodynamics. The first is a unique version
 85 of the first law of quantum thermodynamics, with its def-
 86 inition of quantum heat and quantum work. The second is
 87 a quantum version of Jarzynski's inequality, one that does
 88 not require a two-time measurement scheme. Fifth, the de-
 89 velopment proposes an experiment that highlights geometric
 90 quantum thermodynamics' practical relevance. Finally, it ex-
 91 pands on the geometric approach's increasing relevance to the
 92 thermodynamics of quantum information and computing.

93 II. GEOMETRIC QUANTUM MECHANICS

94 Geometric quantum mechanics arose from efforts to ex-
 95 ploit differential geometry to probe the often-counterintuitive
 96 behaviors of quantum systems. This section summarizes the
 97 relevant concepts, adapting them to our needs. Detailed ex-
 98 positions are found in the original literature [1–18]. Here,
 99 we present the main ideas in a constructive way, focusing
 100 on the aspects that are of direct relevance to thermodynamic
 101 behavior.

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

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

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

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

125 where $Z \in \mathbb{C}^D$, $Z \sim \lambda Z$, and $\lambda \in \mathbb{C}/\{0\}$.

126 For example, the pure state Z_{qubit} of a single qubit can be
 127 given real coordinates: $Z_{\text{qubit}} = (\sqrt{p}, \sqrt{1-p}e^{iv})$. An observ-
 128 able \mathcal{O} is a quadratic real function of the state. It associates
 129 to each point of the pure-state manifold $\mathcal{P}(\mathcal{H})$ the expectation
 130 value $\langle \psi | \mathcal{O} | \psi \rangle$ of the corresponding operator \mathcal{O} on that state:

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

131 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 $K = \ln Z \cdot \bar{Z}$,
 from which one obtains both a metric g :

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

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

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

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 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 ele-
 ment.

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

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

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

(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]

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

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 [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, Hamil-
 tonian 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: $\Omega^{\alpha\gamma} \Omega_{\gamma\beta} = \delta^\alpha_\beta$. Using the symplectic two-form
 one can show that Schrödinger's unitary evolution under op-
 erator 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 other than Hamilton's equa-
 tions of motion in disguise [4,10]:

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

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 [28]. Thus, states are described via functionals $P[\mathcal{O}]$ from the algebra \mathcal{A} of observables to the reals:

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

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 (2) is defined from the Cartesian product measure. Thus,

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

where

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

and

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

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

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

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 them 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

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

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 its 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 $|\psi_{AB}\rangle = \sum_{\alpha,i} \psi_{AB}^{\alpha i} |a_{\alpha}\rangle |b_i\rangle \in \mathcal{H}_{AB}$, 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

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

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

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

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

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

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

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

236 This gives

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

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

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

241 And, eventually, we obtain

$$\rho^A = \sum_{k=1}^{d_B} p_k^A |\chi_k^A\rangle\langle \chi_k^A|, \quad (7)$$

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

$$\mu_{d_B}^A(dZ) := \sum_{k=1}^{d_B} p_k^B \delta_{\chi_k}(dZ),$$

245 where δ_{χ_k} is the Dirac measure with support only on the point
 246 $\chi_k \in \mathcal{P}(\mathcal{H}_A)$ corresponding to the ket $|\chi_k\rangle$.

247 While it is possible to track all information about $\{p_k^A\}_{k=1}^{d_B}$
 248 for small d_B , in the thermodynamic limit this rapidly be-
 249 comes infeasible. A probabilistic description becomes more
 250 appropriate. One could object that this is not a concern since,
 251 at each step in the limit, the spectral decomposition $\rho^A =$
 252 $\sum_{i=1}^{d_A} \lambda_i |\lambda_i\rangle\langle \lambda_i|$, where the λ_i are the Schmidt coefficients of
 253 $|\psi_{AB}\rangle$, is always available. However, this retains only ρ^A 's
 254 matrix elements, erasing the information contained in the
 255 vectors $|v_j\rangle = \sqrt{p_j^A} |\chi_j^A\rangle$. That is, ρ^B has been erased from the
 256 description.

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

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

277 We also imagine that the system’s global dynamics has a
 278 Hamiltonian H_{AB} of fixed functional form: for example, the
 279 XXZ model. Starting with $N_B = N_A$, at each step we add one
 280 repetitive unit $N_B \rightarrow N_B + 1$ and choose a series of pure states
 281 $\{|\psi_{AB}(N_B)\rangle\}_{N_B}$ with the required property that the limit of the
 282 average energy has to be finite:

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

283 For example, one can decide to consistently pick the ground
 284 state of the Hamiltonian H_{AB} . In general, though, there is
 285 no unique way of performing the procedure. However, with
 286 any specific choice of the series $\{|\psi_{AB}(N_B)\rangle\}_{N_B}$ satisfying the
 287 constraint on average energy, the procedure is well defined,
 288 physical, and meaningful. It provides an operational way to
 289 study the thermodynamic limit of the geometric quantum state
 290 $\mu_{d_B}^A$.

291 That said, by no means does this guarantee the limit always
 292 exists. However, it does allow exploring it in a physically
 293 meaningful way. In particular, given this operational imple-
 294 mentation of the thermodynamic limit, we say that

$$\lim_{d_B \rightarrow \infty} \mu_{d_B}^A = \mu_\infty^A.$$

295 This requires a geometric quantum state μ_∞^A on $\mathcal{P}(\mathcal{H}_A)$
 296 such that, for any $\epsilon > 0$ arbitrarily small, one can always
 297 find some finite \bar{d}_B such that for any $d_B \geq \bar{d}_B$ one has
 298 that $D(\mu_{d_B}^A, \mu_\infty^A) \leq \epsilon$. Here, $D(\mu, \nu)$ is a notion of distance
 299 between geometric quantum states that we take to be the
 300 measure-theoretic counterpart of the total variation distance:
 301 $D(\mu, \nu) := \sup_{S \in \mathcal{B}} |\mu(S) - \nu(S)|$, where \mathcal{B} is σ algebra of
 302 $\mathcal{P}(\mathcal{H})$'s Borel sets.

303 When the limit exists, we say that the thermodynamic limit
 304 of the geometric quantum state is μ_∞^A or, equivalently, P_∞^A :

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

305 P_∞^A is a functional whose operational meaning is understood
 306 in terms of ensemble theory, as explained above. Geometric
 307 quantum states describe ensembles of independent and non-
 308 interacting instances of the same quantum system whose pure
 309 states are distributed according to a given probability distribu-
 310 tion. Loosely speaking, if we pick a random pure state out of
 311 the ensemble described by P_∞^A , the probability of finding it in
 312 a small region around Z is $dP_Z = \mu_\infty^A(dZ)$.

313 IV. FROM GEOMETRY TO STATISTICS

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

326 However, one can see how the assumption that all systems
 327 must be in one of the energy eigenstates can be relaxed. After
 328 we extract the k th sample from the macroscopic system, that
 329 sample's state is supposed to be an energy eigenstate $|E_i^{(k)}\rangle$
 330 with probability $p(Z(|E_i^{(k)}\rangle)) \propto e^{-\beta E_i^{(k)}}$. *A priori*, however,
 331 there is no reason to assume that the Hamiltonians H_k of all the
 332 samples are identical to each other. In fact, $|E_i^h\rangle \neq |E_i^k\rangle$ and
 333 $E_i^h \neq E_i^k$. Even if they are, in principle there is no reason why
 334 the qubits should be in their energy eigenstates. This point was
 335 originally made by Khinchin [29] and Schrödinger [30], who
 336 advocated for the use of ensembles of wave functions.

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

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

341 where

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

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

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

344 it also extends this ‘‘Boltzmann’’ rule to arbitrary states:

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

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

in the geometric formalism

$$p_{\text{Gibbs}}(Z) = \sum_{k=0}^{D-1} \frac{e^{-\beta E_k}}{\text{Tr} e^{-\beta H}} \delta[Z - Z(|E_k\rangle)]$$

$$\neq \frac{e^{-\beta h(Z)}}{Q_\beta[h]}.$$

350 This makes explicit the standard formalism's assumption that
 351 the measure is Dirac like: peaked on energy eigenstates.

352 Despite quantum statistical mechanics' undeniable suc-
 353 cesses, this assumption is not, in general, justified. In point
 354 of fact, it is the origin of the missing environmental infor-
 355 mation noted above. These arguments motivate an alternative
 356 formulation of the statistical mechanics of quantum systems,
 357 first introduced in Ref. [19], one based on geometric quantum
 358 states rather than on the familiar density matrices.

359 V. STATISTICAL TREATMENT OF GEOMETRIC 360 QUANTUM MECHANICS

361 Representing a quantum system's state as a continuous
 362 mixed state was first broached, to our knowledge, by Brody
 363 and Hughston [19,20]. Our goal here is to advance the idea,
 364 going from statistical mechanics to thermodynamics. To set
 365 the stage for a *geometric quantum thermodynamics*, the fol-
 366 lowing first presents our version of their results, derived via
 367 the formalism defined in Sec. III, and then expands on them.
 368 We begin with the fundamental postulate of classical statisti-
 369 cal mechanics and its adaptation to quantum mechanics: the
 370 microcanonical and canonical ensembles.

371 A. Classical microcanonical ensemble: *A priori* 372 equal probability

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

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

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

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

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

384 B. Quantum microcanonical ensemble: *A priori* 385 equal probability

386 Quantum statistical mechanics relies on the quantum ver-
 387 sion of the Gibbs ensemble. For macroscopic isolated systems
 388 this is usually interpreted as the quantum system having equal
 389 chance p_{mc} to be in any one of the energy eigenstates $|E_n\rangle$, as

390 long as $E_n \in I_{\text{mc}}$:

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

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

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

395 Geometric quantum mechanics gives an alternative way to ex-
396 tend equal probability to quantum systems, which we discuss
397 now.

398 C. Geometric quantum microcanonical ensemble: *A priori* 399 equal probability

400 The following summarizes an approach to the statisti-
401 cal mechanics of quantum systems first presented in
402 Refs. [19,20,22]. In geometric quantum mechanics the role of
403 the Hamiltonian operator as the generator of unitary dynamics
404 is played by the real quadratic function

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

405 where $H_{\alpha\beta}$ are the matrix elements of the Hamiltonian oper-
406 ator in a reference basis [see Eq. (3)]. As h is the generator
407 of Liouville dynamics on the pure-state manifold $\mathcal{P}(\mathcal{H})$, it is
408 easy to see that there is a straightforward geometric imple-
409 mentation of the *a priori* equal-probability postulate in the
410 quantum setting:

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

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

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

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

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

417 Following Heslot [4], we introduce dimensional coordi-
418 nates via

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

419 where X^α and Y^α are real numbers with dimensions
420 $[X] = [\sqrt{\hbar}] = \text{length}\sqrt{\text{mass}/\text{time}}$ and $[Y] = [\sqrt{\hbar}] =$
421 $\text{momentum}\sqrt{\text{time}/\text{mass}}$. The ratio X/Y is a pure number,
422 while their product XY has the dimension \hbar of an action.
423 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:

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

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

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

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

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

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

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

439 D. Quantum canonical ensemble: Statistical physics 440 of quantum states

441 The geometric approach to microcanonical ensembles ex-
442 tends straightforwardly to the canonical case, defining the
443 continuous canonical ensemble as

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

444 where

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

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

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

451 This is in full agreement with Eq. (6) of Ref. [20].

452 With the ensembles laid out we can now see the emergence
453 of geometric quantum thermodynamics, with its fundamental
454 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 (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

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

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 us 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

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

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:

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

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

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

This gives the standard form of the first law for isothermal, quasistatic processes:

$$dU = T dH_q + dF,$$

where $T := (k_B \beta)^{-1}$. 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 (3) as in classical mechanics:

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

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

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

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

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

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

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

to obtain the second law's familiar form

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

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

536 correlated with its environment. This can be modeled using
 537 the theory of open quantum systems and its dissipative dy-
 538 namics [39–42]. While most approaches focus on establishing
 539 an equation governing the dynamical evolution of the system’s
 540 density matrix, here we are interested in the thermodynamics
 541 of the geometric quantum state as the ensemble behind the
 542 density matrix. A principled description and modeling of the
 543 dynamics of an open quantum system within the geometric
 544 approach is beyond the present scope, although, its develop-
 545 ment is currently ongoing.

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

553 While the emphasis is still on the geometric formalism,
 554 and its natural phase-space geometry, this approach is not far
 555 from “stochastic Schrödinger equations.” See, for example,
 556 Refs. [39,43–46] that import techniques from the classical
 557 theory of stochastic processes. The following exploits this
 558 idea, applying it to the geometric language and drawing from
 559 a variety of known approaches. It does so by examining a
 560 phenomenological model for dissipative dynamics that, as we
 561 show, exhibits thermalization towards the geometric canonical
 562 ensemble.

563 It considers the stochastic dynamics of a two-level sys-
 564 tem with state space $\mathcal{P}(\mathcal{H}) \sim \mathbb{C}P^1$. Generally, this results
 565 from a two-state approximation of a more complex system
 566 interacting with an environment. It gives a standard approxi-
 567 mation that provides sensible results in a variety of physical
 568 regimes. These include systems that inherently consist of
 569 two states, such as spin $\frac{1}{2}$, chiral molecules [47–53], and
 570 atoms at low temperature, considering only the two lowest
 571 states. They also include, though, continuous-variable sys-
 572 tems in a double-well potential, Josephson junctions [54],
 573 and effective descriptions of macroscopic condensates. As a
 574 related technical aside beyond quantum mechanics, we note
 575 that the proper analysis and simulation of stochastic dynam-
 576 ics on Riemannian manifolds is a topic of its own interest
 577 [55,56].

578 Accounting for the nonisolated nature of the system in-
 579 volves modeling the environment and the latter’s effect on
 580 the effective qubit. This, therefore, depends on the specific
 581 case under study and leads to different effective equa-
 582 tions governing the qubit’s nonequilibrium behavior. From
 583 the system’s perspective, however, a general setup is avail-
 584 able in a regime in which coupling with the environment
 585 is weak and the environment is effectively large and dis-
 586 ordered. These approximations are expected to hold for
 587 large environments, where one can argue for the emer-
 588 gence of stochastic dynamics for the evolution of the open
 589 system.

590 The prototypical case, in which a specific form of these
 591 equations can be derived by integrating out the environmental
 592 degrees of freedom, is given by the Caldeira-Leggett model
 593 [57–59] with an environment modeled by an infinite num-
 594 ber of noninteracting harmonic oscillators. Respecting these
 595 approximations’ validity, a generic model of Langevin-type

dynamics on $\mathbb{C}P^1$ is

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

597 in (p, ϕ) coordinates. In this, $E = E(p, \phi)$ is an effective
 598 Hamiltonian generating the deterministic part of the dynamics
 599 [see Eq. (4)]. This is a renormalized version of the system’s
 600 Hamiltonian. V_p and V_ϕ depend linearly on (p, ϕ) and $(\dot{p}, \dot{\phi})$.
 601 They describe (i) dissipative mechanisms such as friction,
 602 modeled with a dependence on \dot{p} or $\dot{\phi}$, as in standard Langevin
 603 equations, and (ii) unstable states, modeled with a dependence
 604 $V_p = -k_p$ to allow for exponential decay $p_{\text{decay}}(t) \sim p_0 e^{-kt}$,
 605 as in a two-level atom decaying into its ground state.

606 Finally, W_p and W_ϕ are stochastic variables with no
 607 drift that account for the environment’s mixing effect on
 608 the system. When the environment is sufficiently large and
 609 unstructured, they can be modeled as Gaussian processes
 610 $\mathbb{E}[W_a(s+t)W_b(s)] = \mathbb{E}[W_a(t)W_b(0)] \approx \delta_{ab}\gamma_a\delta(t)$, with $a, b \in$
 611 $\{p, \phi\}$ and $\gamma_a \propto k_B T$, with T the temperature of the environ-
 612 ment. This is true in the Caldeira-Leggett model for Ohmic
 613 baths.

614 As anticipated above, specific forms of these equa-
 615 tions have successfully modeled the evolution of a variety
 616 of two-level systems. We also note how, in several cases,
 617 and also in Refs. [60–64], this approach to open quantum
 618 systems is quite similar to GQM as it relies on canon-
 619 ical representations of the quantum state space. For chiral
 620 molecules, for example, one has $E(p, \phi) = \delta\langle\sigma_x\rangle + \epsilon\langle\sigma_z\rangle =$
 621 $\delta 2\sqrt{p(1-p)}\cos\phi + \epsilon(1-2p)$, $V_p = -k\dot{p}$, with $k \sim 10^{-1}$,
 622 $W_\phi = V_\phi = 0$ and $W_p(t)$ white noise with strength $\gamma_p \propto k_B T$.
 623 The thermodynamics arising from this set of dynamical equa-
 624 tions has been studied in detail [47–53].

625 The goal here is rather to showcase the experimental rel-
 626 evance of the geometric canonical ensemble. The following
 627 does so showing, numerically, that the evolution provided by
 628 the stochastic equations above leads to the dynamical emer-
 629 gence of the geometric canonical ensemble. This is directly
 630 relevant to the out-of-equilibrium dynamics of an ensemble
 631 of chiral molecules or of an ensemble of experiments with
 632 Josephson junctions.

The specific stochastic equations under study are

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

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

638 Exploiting the Markovian character of Gaussian noise, the
 639 statistics of many independent realizations of this stochastic
 640 process on $\mathbb{C}P^1$ can be extracted by examining the time-
 641 aggregated statistics of a single, very long, trajectory. We thus
 642 simulate the long-time dynamics of a qubit initiated in a fully
 643 out-of-equilibrium configuration $q_0(p, \phi) = \delta(p - p_0)\delta(\phi -$
 644 $\phi_0)$, corresponding to a pure state $|p_0, \phi_0\rangle = \sqrt{1-p_0}|0\rangle +$
 645 $\sqrt{p_0}e^{i\phi_0}|1\rangle$, where $|0\rangle, |1\rangle$ are the standard computational
 646 basis. For chiral molecules, these are the (left and right)

647 chiral eigenstates. Here, we show the results for $p_0 = 0.9$ and
 648 $\phi = 4\pi/3$ and checked that they do not depend on this choice.
 649 Results are shown for parameter values $\delta = \epsilon = 1$, $\gamma = 0.2$,
 650 and $k_d = 0$. While these match the model in Refs. [49,50], the
 651 results are largely independent of this specific choice and hold
 652 for broad regimes in $(\delta, \epsilon, k_d, \gamma)$ parameter space.

653 The analysis was performed as follows. After generating
 654 a single long-time trajectory using the Milstein method, we
 655 collected statistics \tilde{P}_{nk} . We then generated a histogram to ap-
 656 proximate the probability that, at any given time, the system is
 657 found in a small region of the state space $\tilde{P}_{nk} \approx \text{Pr}[Z \in \mathcal{I}_{nk}] =$
 658 $\lim_{T \rightarrow \infty} \int_0^T \int_{\mathcal{I}_{nk}} q_t(Z) dV_{\text{FS}}$. In this, $\{\mathcal{I}_{nk}\}_{n,k=1}^N$ is a coarse
 659 graining of $\mathbb{C}P^1$ in which each region $\mathcal{I}_{nk} = [p_n, p_{n+1}] \times$
 660 $[\phi_k, \phi_{k+1}]$ has the same Fubini-Study volume $\mu_{\text{FS}}(\mathcal{I}_{nk}) =$
 661 N^{-2} , $p_k = n/N$, and $\phi_k = 2\pi k/N$. Reference [33] gives a
 662 detailed analysis of why this is an appropriate coarse graining,
 663 its information-theoretic relevance, and how to generalize it to
 664 arbitrary CP^n .

665 Concretely, the numerical analysis used $N = 50$. The dy-
 666 namics was generated setting $T = 10^2$ in units in which $\hbar =$
 667 $\delta = 1$. This was chosen by numerically checking that the
 668 reconstructed histogram does not change significantly when
 669 increasing T . The time window $[0, T]$ was discretized to
 670 use the Milstein algorithm to generate Gaussian noise with
 671 $dt = 10^{-4}$. These, again, are consistent with the choices in
 672 Refs. [49,50]. In short, the number of time steps $N_T = 10^6$,
 673 with $N_T dt = T$.

674 To extract the inverse temperature β the collected statistics
 675 were used to perform a 2D least-square fit to the geometric
 676 canonical ensemble. The latter's appropriateness was estab-
 677 lished by using the following figure of merit: $f = \sum_{n,k} |\tilde{P}_{nk} -$
 678 $q_{nk}^{\text{fit}}|^2 \in [0, 1]$, where $q_{nk}^{\text{fit}} = Q^{-1} \beta^* \int_{\mathcal{I}_{nk}} dV_{\text{FS}} e^{-\beta^* E(Z)}$ and β^* is
 679 the optimal value extracted from the least-square fit. This is
 680 the total variation distance between the coarse-grained geo-
 681 metric quantum states obtained from the data $\{\tilde{P}_{nk}\}_{n,k}$ and the
 682 one obtained from the best fit to the geometric canonical
 683 ensemble $\{q_{nk}^{\text{fit}}\}_{n,k}$. It ranges from zero to one and is the classical
 684 analog of the well-known trace distance for density matrices.
 685 At selected parameters, $f \approx 5.6 \times 10^{-4}$. This quantifies the
 686 visually excellent agreement seen in Fig. 2.

687 Before drawing broad conclusions, a few comments are in
 688 order regarding specific results. First, thermalization is ob-
 689 served even when changing parameter values. This is true for
 690 any of the Hamiltonian parameters δ and ϵ . Moreover, there
 691 are good numerical indications that this holds for any $k_d > 0$.
 692 However, k_d and γ do affect the effective (inverse) temper-
 693 ature β^* the system reaches. Analyzing how this happens and
 694 the underlying mechanisms is beyond the present scope,
 695 which aimed only at establishing the predictive relevance of
 696 the geometric canonical ensemble in an experimentally realis-
 697 tic setting.

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

703 Third, Eq. (15)'s model arises from a bath that is a set of
 704 noninteracting harmonic oscillators with Ohmic correlation
 705 functions and interactions linear in the phase difference ϕ ,

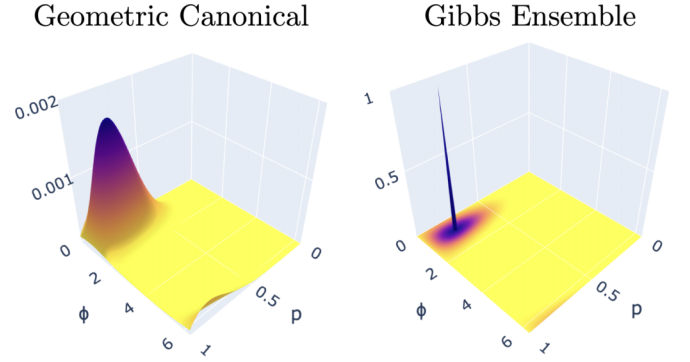


FIG. 1. Alternate ensembles in the geometric and standard
 settings: differences are plainly evident. Canonical probability dis-
 tributions on a qubit's state manifold $\mathbb{C}P^1$ with coordinates $Z =$
 $(Z^0, Z^1) = (\sqrt{1-q}, \sqrt{q}e^{i\chi})$ where $q \in [0, 1]$ and $\chi \in [-\pi, \pi]$.
 $\mathbb{C}P^1$ discretized using a 100×100 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
 $dV_{\text{FS}} = dq d\chi/2$. The Hamiltonian is $H = \sigma_x + \sigma_y + \sigma_z$, with $\hbar =$
 1 and inverse temperature $\beta = 5$ ($k_B = 1$). (Right) Gibbs ensam-
 ble, where the measure is concentrated around 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 en-
 semble. Notice the difference in scale, due to the fact that the
 geometric canonical ensemble has continuous support on the quan-
 tum state space, not just on single points (energy eigenstates).

706 leading to a friction $\propto \dot{\phi}$. A different kind of interaction is
 707 possible, linear in the population p , that leads to a friction term
 708 \dot{p} . While not reported here, there are numerical indications
 709 that this alternative exhibits thermalization to the geometric
 710 canonical ensemble as well. This supports the intuition that
 711 thermalization is mostly driven by the lack of memory of the
 712 stochastic term, ultimately due to the Ohmic nature of the
 713 bath's correlation functions.

714 Fourth, the effective nature of the description makes the
 715 model widely applicable. And so, a number of straightfor-
 716 ward generalizations would be quite interesting to explore.

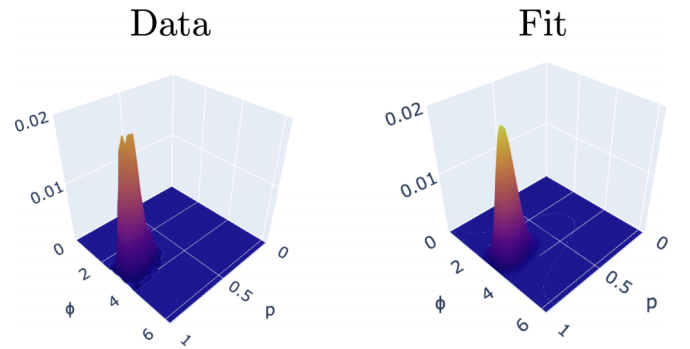


FIG. 2. Comparing time-aggregated data of a single trajec-
 tory generated by Eq. (15)'s stochastic model (left) to the
 fit to a geometric canonical ensemble with functional form
 as in Eq. (9) (right). Here, $h(Z) = E(p, \phi) = \delta(\sigma_x) + \epsilon(\sigma_z) =$
 $\delta 2\sqrt{p(1-p)} \cos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

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 Sec. 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 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 us 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.

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

ACKNOWLEDGMENTS

F.A. thanks A. Ciavarella, M. Radulaski, D. Pastorello, and D. Girolami for discussions on the geometric formalism of quantum mechanics. F.A. and J.P.C. thank D. Gier, D. Karkada, S. Loomis, and A. 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 No. FQXi-RFP-IPW-1902, and U.S. Army Research Laboratory and the [U. S. Army Research Office](#) under Contracts No. W911NF-18-1-0028 and No. W911NF-21-1-0048.

APPENDIX A: INDEPENDENT RESULT

For completeness, the following summarizes the Ref. [31] 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 volumes of the following sets:

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

$$S(\vec{a}, t) := \Delta_n \cap \{\vec{x} \in \mathbb{R}^n : \vec{a}^T \cdot \vec{x} = t\},$$

where \vec{a}^T is the transpose of \vec{a} . The result assumes flat geometry, which is obtained from the volume element

826 $dp_1 dp_2 \dots dp_n$. Letting $(x)_+ := \max(0, x)$ and $a_0 = 0$, then

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

827 and

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

828 **APPENDIX B: GEOMETRIC QUANTUM DENSITY**
829 **OF STATES AND CANONICAL ENSEMBLE**

830 Again for completeness, we first recall the basic defini-
831 tions, given in the main text, used in the two sections that
832 follow to calculate the density of states and statistical physics
833 of quantum states in the geometric formalism.

834 **1. Setup and notation**

835 Consider a Hilbert space \mathcal{H} of finite dimension D . The
836 manifold $\mathcal{P}(\mathcal{H})$ of states is the complex projective space
837 $\mathbb{C}P^{D-1}$. A point Z on the manifold is a set of D homogeneous
838 and complex coordinates $\{Z^\alpha\}$. A point corresponds to a pure
839 state with the identification $Z \leftrightarrow |\psi\rangle = \sum_{\alpha=0}^{D-1} Z^\alpha |e_\alpha\rangle$, where
840 $\{|e_\alpha\rangle\}_\alpha$ is an arbitrary but fixed basis of \mathcal{H} . This parametriza-
841 tion underlies the choice of a reference basis that, however,
842 is ultimately irrelevant. While concrete calculations of exper-
843 imentally measurable quantities can be made easier or harder
844 by an appropriate coordinate system, the overall result is
845 independent on such choices. The quantum mechanical expecta-
846 tion value is a quadratic and real function on the manifold
847 of the quantum states:

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

848 When $A = H$ is the system's Hamiltonian, the function
849 $a(Z) = h(Z)$ generates the vector field V_H on $\mathbb{C}P^{D-1}$. The
850 associated Hamiltonian equations of motion become the
851 Schrödinger equation (and its complex conjugate) when using
852 the standard formalism with Hilbert spaces. In the geometric
853 formalism, states are functionals from the algebra of observ-
854 ables to the real numbers. Effectively, they are probability
855 distributions, both discrete and continuous, on the quantum-
856 state manifold $\mathbb{C}P^{D-1}$.

2. Microcanonical density of states: Proof of Eq. (8) 857

We start with the *a priori* equal-probability postulate and
858 build the microcanonical shell as follows: 859

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

860 Due to normalization we have

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

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

$$dV_{\text{FS}} = \frac{1}{2^n} dp_1 dp_2 \dots dp_n dv_1 \dots dv_n.$$

862 This gives the manifold volume

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

863 For concrete calculations, normalize the measure so that
864 $\mathbb{C}P^{D-1}$'s total volume is unity, using

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

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

869 We can now compute $W(\mathcal{E})$ for a generic quantum sys-
870 tem. Assuming that $\delta\mathcal{E} \ll |E_{\text{max}} - E_{\text{min}}|$, we have $W(\mathcal{E}) =$
871 $\Omega(\mathcal{E})\delta\mathcal{E}$ and $\Omega(\mathcal{E})$ is the area of the surface Σ defined by
872 $h(Z) = \mathcal{E}$:

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

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

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

877 adapted to the surface Σ :

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

878 On both sides we subtract the ground-state energy E_0
879 and divide by $E_{\text{max}} - E_0$ to obtain the following defining

880 equation for $\Sigma \subset \mathbb{C}P^n$:

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

881 with

$$\varepsilon_k = \frac{E_k - E_0}{E_{\max} - E_0} \in [0, 1] \text{ and}$$

$$\varepsilon = \frac{\mathcal{E} - E_0}{E_{\max} - E_0} \in [0, 1].$$

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

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

883 where $n_k \in [0, 1]$ and $\nu_k \in [0, 2\pi[$. With the transformation
884 $p_k = n_k^2$ the equation for Σ becomes

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

885 **a. Qubit case**

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

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

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

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

890 In turn, this gives

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

891 In other words,

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

892 which is a constant density of states.

893 **b. Qutrit case**

894 The state space of qutrits is $\mathbb{C}P^2$, with parametriza-
895 tion $Z = (Z_0, Z_1, Z_2) = (1-p-q, pe^{i\nu_1}, qe^{i\nu_2})$. With these
896 coordinates, the equation defining the constant-energy hyper-
897 surface is

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

898 And, it has volume

$$\text{Vol}_{n=2}(\mathcal{E}) = \frac{2}{(2\pi)^2} \int \int dq dq \int \int d\nu_1 d\nu_2$$

$$= 2 \int \int_S dp dq.$$

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
899 that the region's area is
900
901

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

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
902 are continuous. Eventually, we have
903
904

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

905 **c. Generic qudit case: $\mathbb{C}P^n$**

To use the Ref. [31] result, summarized in Appendix A, we
906 must change coordinates. Again, using “probability + phase”
907 coordinates
908

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

means that

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

$$R = \sqrt{\sum_{k=1}^n (E_k - E_0)^2}, \text{ and}$$

$$t(\mathcal{E}) = \frac{\mathcal{E} - E_0}{R}.$$

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 exists 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
910 at $k = \bar{n}$ because after that $(\mathcal{E} - E_k)_+ = 0$. Hence, there exists
911 $\bar{n}(\mathcal{E})$ such that for all $k > \bar{n}$ we have $(\mathcal{E} - E_k)_+ = 0$. This, in
912 turn, shows that
913
914
915

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

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

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

918 This allows defining the *statistical entropy* $S(\mathcal{E})$ of a quantum
 919 system with finite-dimensional Hilbert space of dimension
 920 $D = n + 1$ as

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

921 3. Statistical physics of quantum states: Canonical ensemble

922 The continuous canonical ensemble is defined as

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

923 where

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

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

927 a. Single qubit

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

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

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

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

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

936 Or, using “probability + phase” coordinates (p, ν) we can also
 937 write

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

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

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

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

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

$$Q_\beta[h] = \int_{\mathbb{C}P^n} e^{-\beta h(Z)} dV_{\text{FS}}$$

$$= \frac{1}{2^n} \int \prod_{k=0}^n e^{-\beta p_k E_k} \prod_{k=1}^n dp_k d\nu_k \\ = \pi^n \int_{\Delta_n} \prod_{k=0}^n e^{-\beta p_k E_k} \delta\left(\sum_{k=0}^n p_k - 1\right) dp_1 \dots dp_n.$$

To evaluate the integral we first take the Laplace transform 943

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

to get 944

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

Calculating, we find 945

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

with $z_k = -\beta E_k \in \mathbb{R}$. 946

The function $\tilde{I}_n(z)$ has $n + 1$ real and distinct poles: $z =$ 947
 $z_k = -\beta E_k$. Hence, we can exploit the partial fraction decom- 948
 position of $\tilde{I}_n(z)$, which is 949

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

where 950

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

The inverse Laplace transform’s linearity, coupled with the 951
 basic result 952

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

where 953

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

gives 954

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

And so, we finally see that 955

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

- [1] F. Strocchi, Complex Coordinates and Quantum Mechanics, *Rev. Mod. Phys.* **38**, 36 (1966).
- [2] T. W. B. Kibble, Geometrization of Quantum Mechanics, *Commun. Math. Phys.* **65**, 189 (1979).
- [3] P. R. Chernoff and J. E. Marsden, Some remarks on Hamiltonian systems and quantum mechanics, in *Foundations of Probability Theory, Statistical Inference, and Statistical Theories of Science* (Springer, Berlin, 1976), Vol. III, pp. 35–53.
- [4] A. Heslot, Quantum mechanics as a classical theory, *Phys. Rev. D* **31**, 1341 (1985).
- [5] G. W. Gibbons, Typical states and density matrices, *J. Geom. Phys.* **8**, 147 (1992).
- [6] A. Ashtekar and T. A. Schilling, Geometry of quantum mechanics, in *AIP Conference Proceedings*, Volume 342 (AIP, Woodbury, NY, 1995), pp. 471–478.
- [7] A. Ashtekar and T. A. Schilling, Geometrical formulation of quantum mechanics, in *On Einstein's Path* (Springer, New York, 1999), pp. 23–65.
- [8] L. P. Hughston, Geometric aspects of quantum mechanics, in *Twistor Theory*, Lecture Notes in Pure and Applied Mathematics, Vol. 169, edited by Stephen Huggett (Marcel Dekker, New York, 1995), Chap. 6.
- [9] D. C. Brody and L. P. Hughston, Geometric quantum mechanics, *J. Geom. Phys.* **38**, 19 (2001).
- [10] I. Bengtsson and K. Życzkowski, *Geometry of Quantum States* (Cambridge University Press, Cambridge, 2017).
- [11] J. F. Cariñena, J. Clemente-Gallardo, and G. Marmo, Geometrization of Quantum Mechanics, *Theor. Math. Phys.* **152**, 894 (2007).
- [12] D. Chruściński, Geometric Aspects of Quantum Mechanics and Quantum Entanglement, *J. Phys.: Conf. Ser.* **30**, 9 (2006).
- [13] G. Marmo and G. F. Volkert, Geometrical description of quantum mechanics—transformations and dynamics, *Phys. Scr.* **82**, 038117 (2010).
- [14] J. Avron and O. Kenneth, An elementary introduction to the geometry of quantum states with pictures, *Rev. Math. Phys.* **32**, 2030001 (2020).
- [15] D. Pastorello, A geometric Hamiltonian description of composite quantum systems and quantum entanglement, *Int. J. Geom. Methods Mod. Phys.* **12**, 1550069 (2015).
- [16] D. Pastorello, Geometric Hamiltonian formulation of quantum mechanics in complex projective spaces, *Int. J. Geom. Methods Mod. Phys.* **12**, 1560015 (2015).
- [17] D. Pastorello, Geometric Hamiltonian quantum mechanics and applications, *Int. J. Geom. Methods Mod. Phys.* **13**, 1630017 (2016).
- [18] J. Clemente-Gallardo and G. Marmo, The Ehrenfest Picture and the Geometry of Quantum Mechanics, *Nuovo Cimento C* **3**, 35 (2013).
- [19] D. C. Brody and L. P. Hughston, The quantum canonical ensemble, *J. Math. Phys.* **39**, 6502 (1998).
- [20] D. C. Brody, D. W. Hook, and L. P. Hughston, On quantum microcanonical equilibrium, *J. Phys.: Conf. Ser.* **67**, 012025 (2007).
- [21] D. C. Brody and L. P. Hughston, Thermodynamics of quantum heat bath, *J. Phys. A: Math. Theor.* **49**, 425302 (2016).
- [22] D. C. Brody, D. W. Hook, and L. P. Hughston, Quantum phase transitions without thermodynamic limits, *Proc. R. Soc. A: Math. Phys. Eng. Sci.* **463**, 2021 (2007).
- [23] U. Seifert, Stochastic thermodynamics: Principles and perspectives, *Eur. Phys. J. B* **64**, 423 (2008).
- [24] U. Seifert, Stochastic thermodynamics, fluctuation theorems and molecular machines, *Rep. Prog. Phys.* **75**, 126001 (2012).
- [25] J. Gemmer, M. Michel, and G. Mahler, *Quantum Thermodynamics*, Volume 657 of Lecture Notes in Physics (Springer, Berlin, 2004).
- [26] S. Deffner and S. Campbell, *Quantum Thermodynamics*, (IOP Publishing, Bristol, UK, 2019).
- [27] F. Anza and J. P. Crutchfield, Beyond density matrices: Geometric quantum states, *Phys. Rev. A* **103**, 062218 (2021).
- [28] F. Strocchi, *An Introduction to the Mathematical Structure of Quantum Mechanics: A Short Course for Mathematicians* (World Scientific, Singapore, 2008).
- [29] Khinchin, *Mathematical Foundations of Quantum Statistics* (Dover, New York, 1951).
- [30] E. Schrödinger, *Statistical Thermodynamics* (Cambridge University Press, Cambridge, 1952).
- [31] J. B. Lasserre, Volume of slices and sections of the simplex in closed form, *Optim. Lett.* **9**, 1263 (2015).
- [32] D. C. Brody and L. P. Hughston, Information content for quantum states, *J. Math. Phys.* **41**, 2586 (2000).
- [33] F. Anza and J. P. Crutchfield, Quantum information dimension and geometric entropy, *PRX Quantum* **3**, 020355 (2022).
- [34] G. E. Crooks, Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences, *Phys. Rev. E* **60**, 2721 (1999).
- [35] C. Jarzynski, Equalities and Inequalities: Irreversibility and the Second Law of Thermodynamics at the Nanoscale, *Annu. Rev. Condens. Matter Phys.* **2**, 329 (2011).
- [36] M. Campisi, P. Hänggi, and P. Talkner, Colloquium: Quantum fluctuation relations: Foundations and applications, *Rev. Mod. Phys.* **83**, 771 (2011).
- [37] R. Klages, W. Just, and C. Jarzynski, *Nonequilibrium Statistical Physics of Small Systems: Fluctuation Relations and Beyond* (Wiley-VCH, Weinheim, 2013).
- [38] C. Jarzynski, Nonequilibrium Equality for Free Energy Differences, *Phys. Rev. Lett.* **78**, 2690 (1997).
- [39] H. P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002).
- [40] U. Weiss, *Quantum Dissipative Systems* (World Scientific, Singapore, 2012).
- [41] C. Gardiner and P. Zoller, *Quantum Noise* (Springer, Berlin, 2010).
- [42] H. Carmichael, *An Open Systems Approach to Quantum Optics* (Springer, Berlin, 1993).
- [43] L. Bouten, M. Guta, and H. Maassen, Stochastic Schrödinger equations, *J. Phys. A: Math. Gen.* **37**, 3189 (2004).
- [44] V. P. Belavkin, A new wave equation for a continuous nondemolition measurement, *Phys. Lett. A* **140**, 355 (1989).
- [45] V. P. Belavkin, A continuous counting observation and posterior quantum dynamics, *J. Phys. A: Math. Gen.* **22**, L1109 (1989).
- [46] V. P. Belavkin, Nondemolition measurements, nonlinear filtering and dynamic programming of quantum stochastic processes, in *Proceedings of Bellmann Continuum Workshop on Modelling and Control of Systems*, Volume 121 of Lecture Notes in Control and Information Science (Springer, Berlin, 1988).
- [47] A. Dorta-Urra, H. C. Penate-Rodríguez and P. Bargueno, G. Rojas-Lorenzo, and S. Miret-Artes, Dissipative geometric

- phase and decoherence in parity-violating chiral molecules, *J. Chem. Phys.* **136**, 174505 (2012).
- [48] P. Bargaño, H. C. Penate-Rodríguez, I. Gonzalo, F. Sols, and S. Miret-Artes, Friction-induced enhancement in the optical activity of interacting chiral molecules, *Chem. Phys. Lett.* **516**, 29 (2011).
- [49] H. C. Peñate-Rodríguez, A. Dorta-Urra, P. Bargaño, and G. Rojas-Lorenzo, A Langevin canonical approach to the dynamics of chiral systems: Thermal averages and heat capacity, *Chirality* **26**, 319 (2014).
- [50] H. C. Peñate-Rodríguez, A. Dorta-Urra, P. Bargaño, and G. Rojas-Lorenzo, A Langevin canonical approach to the dynamics of chiral systems: Populations and coherences, *Chirality* **25**, 514 (2013).
- [51] P. Bargaño and S. Miret-Artes, Dissipative and stochastic geometric phase of a qubit within a canonical Langevin framework, *Phys. Rev. A* **87**, 012125 (2013).
- [52] P. Bargaño and S. Miret-Artes, The generalized Schrödinger-Langevin equation, *Ann. Phys.* **346**, 59 (2014).
- [53] R. Katz and P. B. Gossiaux, The Schrödinger-Langevin equation with and without thermal fluctuations, *Ann. Phys.* **368**, 267 (2016).
- [54] R. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics, Volume 3* (Addison-Wesley, Reading, MA, 1963).
- [55] A. V. Gómez and F. J. Sevilla, A geometrical method for the Smoluchowski equation on the sphere, *J. Stat. Mech.* (2021) 083210.
- [56] P. H. Roberts and H. D. Ursell, Random walk on a sphere and on a Riemannian manifold, *Philos. Trans. R. Soc. London A* **252**, 196 (1960).
- [57] A. O. Caldeira and A. J. Leggett, Path integral approach to quantum brownian motion, *Phys. A (Amsterdam)* **121**, 587 (1983).
- [58] A. O. Caldeira and A. J. Leggett, Quantum tunnelling in a dissipative system, *Ann. Phys.* **149**, 374 (1983).
- [59] A. J. Leggett, S. Chakravarty, A. T. Dorsey, Matthew P. A. Fisher, Anupam Garg, and W. Zwerger, Dynamics of the dissipative two-state system, *Rev. Mod. Phys.* **59**, 1 (1987).
- [60] W. H. Miller and C. W. McCurdy, Classical trajectory modeling for electronically nonadiabatic collision phenomena. a classical analog for electronic degrees of freedom, *J. Chem. Phys.* **69**, 5163 (1978).
- [61] H.-D. Meyer and C. W. McCurdy, A classical analog for electronic degrees of freedom in nonadiabatic collision processes, *J. Chem. Phys.* **70**, 3214 (1979).
- [62] M. D. Kostin, On the Schrödinger-Langevin equation, *J. Chem. Phys.* **57**, 3589 (1972).
- [63] G. Stock and M. Thoss, Semiclassical Description of Nonadiabatic Quantum Dynamics, *Phys. Rev. Lett.* **78**, 578 (1997).
- [64] D. Chruszinsky and A. Jamiolkovsky, *Geometric Phases in Classical and Quantum Mechanics*, Progress in Mathematical Physics (Birkhauser, Basel, 2004).
- [65] M. Campisi, Quantum fluctuation relations for ensembles of wave functions, *New J. Phys.* **15**, 115008 (2013).