

UC Davis

UC Davis Previously Published Works

Title

Beyond density matrices: Geometric quantum states

Permalink

<https://escholarship.org/uc/item/83j9q3np>

Journal

Physical Review A, 103(6)

ISSN

2469-9926

Authors

Anza, Fabio
Crutchfield, James P

Publication Date

2021-06-01

DOI

10.1103/physreva.103.062218

Peer reviewed

Beyond Density Matrices: Geometric Quantum States

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)

A quantum system’s state is identified with a density matrix. Though their probabilistic interpretation is rooted in ensemble theory, density matrices embody a known shortcoming. They do not completely express an ensemble’s physical realization. Conveniently, when working only with the statistical outcomes of projective and positive operator-valued measurements this is not a hindrance. To track ensemble realizations and so remove the shortcoming, we explore geometric quantum states and explain their physical significance. We emphasize two main consequences: one in quantum state manipulation and one in quantum thermodynamics.

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

Keywords: Quantum Mechanics, Geometric Quantum Mechanics

Introduction. Dynamical systems theory describes long-term recurrent behavior via a system’s *attractors*: stable dynamically-invariant sets. Said simply there are regions of state space—points, curves, smooth manifolds, or fractals—the system repeatedly visits. These objects are implicitly determined by the underlying equations of motion and are modeled as probability distributions (measures) on the system’s state space.

Building on this, the following introduces tools aimed at studying attractors for quantum systems. This requires developing a more fundamental concept of “state of a quantum system”, essentially moving beyond the standard notion of density matrices, though they can be directly recovered. We call these objects the system’s *geometric quantum states* and, paralleling the Sinai-Bowen-Ruelle measures of dynamical systems theory [1], they are specified by a probability distribution on the manifold of quantum states.

Quantum mechanics is firmly grounded in a vector formalism in which states $|\psi\rangle$ are elements of a complex Hilbert space \mathcal{H} . These are the system’s *pure states*, as opposed to *mixed states* that account for incomplete knowledge of a system’s actual state. To account for both, one employs *density matrices* ρ . These are operators in \mathcal{H} that are positive semi-definite $\rho \geq 0$, self-adjoint $\rho = \rho^\dagger$, and normalized $\text{Tr } \rho = 1$.

The interpretation of a density matrix as a system’s *probabilistic state* is given by *ensemble theory* [2, 3]. Accordingly, since a density matrix always decomposes into eigenvalues λ_i and eigenvectors $|\lambda_i\rangle$:

$$\rho = \sum_i \lambda_i |\lambda_i\rangle \langle \lambda_i| , \quad (1)$$

one interprets ρ as an ensemble of pure states—the eigenvectors—in which λ_i is the probability of an observer interacting with state $|\lambda_i\rangle$.

However, this interpretation is problematic: It is not unique. One can write the same ρ using different decompositions, for example in terms of $\{|\psi_k\rangle\} \neq \{|\lambda_i\rangle\}$:

$$\rho = \sum_k p_k |\psi_k\rangle \langle \psi_k| .$$

Given the interpretation, all the decompositions identify the same quantum state ρ . While one often prefers Eq. (1)’s diagonal decomposition in terms of eigenvalues and eigenvectors, it is not the only one possible. More tellingly, in principle, there is no experimental reason to prefer it to others. In quantum mechanics, this fact is often addressed by declaring density matrices with the same *barycenter* equal. A familiar example of this degeneracy is that the maximally mixed state ($\rho \propto \mathbb{I}$) has an infinite number of identical decompositions, each possibly representing a physically-distinct ensemble.

Moreover, it is rather straightforward to construct systems that, despite having the same density matrix, are in different states. For example, consider two distinct state-preparation protocols. In one case, prepare states $\{|0\rangle, |1\rangle\}$ each with probability 1/2; while, in the other, always prepare states $\{|-\rangle, |+\rangle\}$ each with probability 1/2. They are described by the same ρ . A complete and unambiguous mathematical concept of state should not conflate distinct physical configurations. Not only do such ambiguities lead to misapprehending fundamental mechanisms, they also lead one to ascribe complexity where there is none.

Here we argue that an alternative—the *geometric formalism*—together with an appropriately adapted measure theory cleanly separates the primary concept of a *system state* from the derived concept of a density matrix as the set of all *positive operator-valued measurement statistics* generated by a system.

With this perspective in mind, we introduce a more incisive description of pure-state ensembles. The following argues that *geometric quantum mechanics* (GQM), through its notion that geometric quantum states are *continuous mixed states*, resolves the ambiguities. First, we introduce

* fanza@ucdavis.edu

† chaos@ucdavis.edu

GQM. Second, we discuss how it relates to the density matrix formalism. Then we analyze two broad settings in which the geometric formalism arises quite naturally: quantum state manipulation [4] and quantum thermodynamics [5]. After discussing the results, we draw out several consequences.

Geometric quantum mechanics. References [6–21] give a comprehensive introduction to GQM. Here, we briefly summarize only the elements we need, working with Hilbert spaces \mathcal{H} of finite dimension D .

Pure states are points in the complex projective manifold $\mathcal{P}(\mathcal{H}) = \mathbb{C}\mathbb{P}^{D-1}$. Therefore, given an arbitrary basis $\{|e_\alpha\rangle\}_{\alpha=0}^{D-1}$, a pure state ψ is parametrized by D complex homogeneous coordinates $Z = \{Z^\alpha\}$, 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 $\lambda \in \mathbb{C}/\{0\}$. If the system consists of a single qubit, for example, one can always use amplitude-phase coordinates $Z = (\sqrt{1-p}, \sqrt{p}e^{i\nu})$.

An *observable* is a quadratic real function $\mathcal{O}(Z) \in \mathbb{R}$ that associates to each point $Z \in \mathcal{P}(\mathcal{H})$ the expectation value $\langle \psi | \mathcal{O} | \psi \rangle$ of the corresponding operator \mathcal{O} on state $|\psi\rangle$ with coordinates Z :

$$\mathcal{O}(Z) = \sum_{\alpha,\beta} \mathcal{O}_{\alpha,\beta} Z^\alpha \bar{Z}^\beta , \quad (2)$$

where $\mathcal{O}_{\alpha\beta}$ is Hermitian $\mathcal{O}_{\beta,\alpha} = \overline{\mathcal{O}_{\alpha,\beta}}$.

Measurement outcome probabilities are determined by *positive operator-valued measurements* (POVMs) $\{E_j\}_{j=1}^n$ applied to a state [22, 23]. They are nonnegative operators $E_j \geq 0$, called *effects*, that sum up to the identity: $\sum_{j=1}^n E_j = \mathbb{I}$. In GQM they consist of nonnegative real functions $E_j(Z) \geq 0$ on $\mathcal{P}(\mathcal{H})$ whose sum is always unity:

$$E_j(Z) = \sum_{\alpha,\beta} (E_j)_{\alpha,\beta} Z^\alpha \bar{Z}^\beta , \quad (3)$$

where $\sum_{j=1}^n E_j(Z) = 1$.

Complex projective spaces, such as $\mathcal{P}(\mathcal{H})$, have a preferred metric g_{FS} —the *Fubini-Study metric* [13]—and an associated volume element dV_{FS} that is coordinate-independent and invariant under unitary transformations. The geometric derivation of dV_{FS} is beyond our immediate goals here. That said, it is sufficient to give its explicit form in the “probability + phase” coordinate system $Z^\alpha = \sqrt{p_\alpha} e^{i\nu_\alpha}$ that we use for explicit calculations:

$$\begin{aligned} dV_{FS} &= \sqrt{\det g_{FS}} \prod_{\alpha=0}^{D-1} dZ^\alpha d\bar{Z}^\alpha \\ &= \prod_{\alpha=1}^{D-1} \frac{dp_\alpha d\nu_\alpha}{2} . \end{aligned}$$

Notice how p_0 and ν_0 are not involved. This is due to $\mathcal{P}(\mathcal{H})$ ’s projective nature which guarantees that we can choose a coordinate patch in which $p_0 = 1 - \sum_{\alpha=1}^{D-1} p_\alpha$ and $\nu_0 = 0$.

Geometric quantum states. This framework makes it very natural to view a quantum state as a functional encoding that associates expectation values to observables, paralleling the C^* -algebras formulation of quantum mechanics [24]. Thus, states are described as functionals $P[\mathcal{O}]$ from the algebra of observables \mathcal{A} to the real line:

$$P_q[\mathcal{O}] = \int_{\mathcal{P}(\mathcal{H})} q(Z) \mathcal{O}(Z) dV_{FS} , \quad (4)$$

where $\mathcal{O} \in \mathcal{A}$, $q(Z) \geq 0$ is the normalized distribution associated with functional P :

$$P_q[\mathbb{I}] = \int_{\mathcal{P}(\mathcal{H})} q(Z) dV_{FS} = 1 ,$$

and $P_q[\mathcal{O}] \in \mathbb{R}$.

In this way, pure states $|\psi_0\rangle$ are functionals with a Dirac-delta distribution $p_0(Z) = \tilde{\delta}[Z - Z_0]$:

$$\begin{aligned} P_0[\mathcal{O}] &= \int_{\mathcal{P}(\mathcal{H})} \tilde{\delta}(Z - Z_0) \mathcal{O}(Z) dV_{FS} \\ &= \mathcal{O}(Z_0) = \langle \psi_0 | \mathcal{O} | \psi_0 \rangle . \end{aligned}$$

$\tilde{\delta}(Z - Z_0)$ is shorthand for a coordinate-covariant Dirac-delta in arbitrary coordinates. In homogeneous coordinates this reads:

$$\tilde{\delta}(Z - Z_0) := \frac{1}{\sqrt{\det g_{FS}}} \prod_{\alpha=0}^{D-1} \delta(X - X_0) \delta(Y - Y_0) ,$$

where $Z = X + iY$. In (p_α, ν_α) coordinates this becomes simply:

$$\tilde{\delta}(Z - Z_0) = \prod_{\alpha=1}^{D-1} 2\delta(p_\alpha - p_\alpha^0) \delta(\nu_\alpha - \nu_\alpha^0) , \quad (5)$$

where the coordinate-invariant nature of the functionals $P_q[\mathcal{O}]$ is now apparent.

In this way, too, mixed states:

$$\rho = \sum_j \lambda_j |\lambda_j\rangle \langle \lambda_j|$$

are convex combinations of these Dirac-delta functionals:

$$q_{\text{mix}}(Z) = \sum_j \lambda_j \tilde{\delta}(Z - Z_j) .$$

Thus, expressed as functionals from observables to the

real line, mixed states are:

$$P_{\text{mix}}[\mathcal{O}] = \sum_j \lambda_j \langle \lambda_j | \mathcal{O} | \lambda_j \rangle . \quad (6)$$

Equipped with this formalism, one identifies the distribution $q(Z)$ as a system's *geometric quantum state*. This is the generalized notion of quantum state we develop in the following.

A simple example of an ensemble that is neither a pure nor a mixed state is the *geometric canonical ensemble*:

$$q(Z) = \frac{1}{Q_\beta} e^{-\beta h(Z)} ,$$

where:

$$Q_\beta = \int dV_{FS} e^{-\beta h(Z)} ,$$

$$h(Z) = \langle \psi(Z) | H | \psi(Z) \rangle ,$$

and H is the system's Hamiltonian operator. This state was previously considered in Refs. [25, 26]. Reference [5] investigated its potential role in establishing a quantum foundation of thermodynamics that is an alternative to that based on Gibbs ensembles and von Neumann entropy. Moreover, it showed that the geometric ensemble genuinely differs from the Gibbs ensemble. This realization provides a concrete path to testing the experimental consequences of geometric quantum states.

Density matrix. The connection between geometric quantum states and density matrices is two-fold. On the one hand, when the distribution $q(Z)$ falls into one of the two aforementioned cases—Dirac-deltas or finite convex combinations of them—the present formalism is equivalent to the standard one. However, not all functionals fall into the Dirac-delta form. Given this, $q(Z)$ is clearly a more general notion of a quantum system's state.

On the other hand, given an arbitrary distribution $q(Z)$, there is a unique density matrix ρ^q associated to q :

$$\rho_{\alpha\beta}^q = P_q[Z^\alpha \bar{Z}^\beta]$$

$$= \int_{\mathcal{P}(\mathcal{H})} dV_{FS} q(Z) Z^\alpha \bar{Z}^\beta . \quad (7)$$

Owing it to the fact that all POVMs are represented by real and quadratic functions on $\mathcal{P}(\mathcal{H})$, recall Eq. (3), they are sensitive to $q(Z)$ via ρ^q . Therefore, if two distributions q_1 and q_2 induce the same density matrix $\rho^{q_1} = \rho^{q_2}$, then all POVMs produce the same outcomes.

A well-known consequence of this fact is that two density matrices with the same barycenter are considered equal, even if they describe experiments with different physical configurations. In these cases, the statistics of POVM outcomes are described by the same density matrix. Note that this statement does not mean that the two systems are in the same *state*. Rather, it means that there is no

POVM on the system that distinguishes between q_1 and q_2 .

To emphasize, consider the example of two geometric quantum states, q_1 and q_2 , with very different characteristics:

$$q_1(Z) = \frac{1}{Q} e^{-\frac{1}{2} Z \bar{\rho}^{-1} Z}$$

$$q_2(Z) = 0.864 \tilde{\delta}(Z - Z_+) + 0.136 \tilde{\delta}(Z - Z_-) ,$$

where $Q = \int_{\mathbb{C}P^1} dV_{FS} e^{-\frac{1}{2} Z \bar{\rho}^{-1} Z}$, $Z_+ = (0.657, 0.418 + i0.627)$, and $Z_- = (0.754, -0.364 - i0.546)$. However, states q_1 and q_2 have same density matrix ρ ($\rho_{00} = 0.45 = 1 - \rho_{11}$ and $\rho_{01} = 0.2 - i0.3 = \rho_{10}^*$) and so the same POVM outcomes. From Fig.1 one appreciates the profound difference between q_1 and q_2 , despite the equality of their POVM statistics.

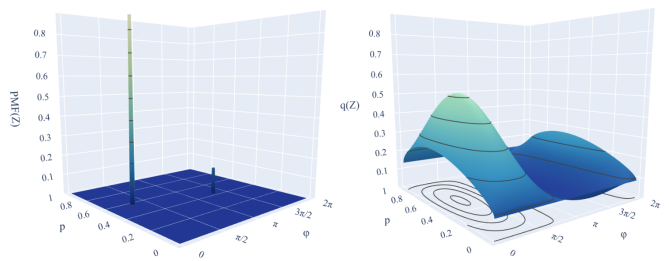


Figure 1. Geometric quantum states in $(probability, phase)$ coordinates (p, ϕ) of $\mathbb{C}P^1$: (Left) Density matrix “state” q_1 is the convex sum of two Dirac delta-functions, centered on the eigenvectors $(p_+, \phi_+) = (0.568, 0.983)$ and $(p_-, \phi_-) = (0.432, 4.124)$ of density matrix ρ . (Right) Geometric quantum state q_2 differs markedly: A smooth distribution across the entire pure-state manifold $\mathbb{C}P^1$. However, q_1 and q_2 have the same density matrix $\rho_{q_1} = \rho_{q_2} = \rho$, where $\rho_{00} = 1 - \rho_{11} = 0.45$, $\rho_{01} = \rho_{10}^* = 0.2 - 0.3i$. ρ_{\pm} are the eigenvalues of the density matrix: $\rho_+ = 0.864$ and $\rho_- = 0.136$. Geometric quantum state q_2 's structure is only sparsely reflected in the density-matrix “state” q_1 .

This is particularly important for quantum information processing where one encounters long-range and long-lived correlational and mechanistic demands. Quantum computing immediately comes to mind. There, one is not only interested in measurement outcomes, but also in predicting and understanding how a quantum system evolves under repeated external manipulations imposed by complex control protocols.

State manipulation. The following shows that the geometric formalism arises quite naturally when a discrete quantum system interacts and develops entanglement with a continuous one. Imagine a protocol controlling a system's continuous degrees of freedom to manipulate discrete ones that store a computation's result. As a physical reference, consider quantum particles with a given number of discrete degrees of freedom (e.g., spin), confined to a region $\mathcal{R} \subseteq \mathbb{R}^3$. The results we derive do not depend on this choice, since the technical methods straightforwardly

extend to other systems where continuous and discrete degrees of freedom are mixed. A helpful illustration is intra-particle entanglement [27], that couples position and spin degrees of freedom to create entangled states. In this way, one manipulates the spin by only acting on the positional degrees of freedom, possibly via a potential.

Consider a hybrid quantum system comprised of N continuous degrees of freedom and M qudits that are the discrete ones. The entire system's Hilbert space is:

$$\mathcal{H} = \mathcal{H}_N^c \otimes \mathcal{H}_M^d,$$

where \mathcal{H}_N^c hosts the continuous degrees of freedom and has infinite dimension, while \mathcal{H}_M^d hosts the discrete ones and has dimension d^M . A basis for \mathcal{H}_N^c is provided by $\{|\vec{x}\rangle\}$, where $\vec{x} \in \mathcal{R} \subseteq \mathbb{R}^N$ and a basis for \mathcal{H}_M^d is $\{|s\rangle\}_{s=0}^{d^M-1}$. Thus, a generic state is:

$$|\psi\rangle = \int_{\mathcal{R}} d\vec{x} \sum_s \psi_s(\vec{x}) |\vec{x}\rangle |s\rangle,$$

where \vec{x} is a dimensionless counterpart of the physical continuous degrees of freedom, achieved by multiplying its value by appropriate physical quantities. So, the measure $d\vec{x}$ has no physical dimension. For an electron in a box, for example, this is achieved by renormalizing with the box's total volume.

The following theorem establishes that this can be done constructively.

Theorem 1. *Any state $|\psi\rangle \in \mathcal{H}$ can be written as:*

$$|\psi\rangle = \int_{\mathcal{R}} d\vec{x} f(\vec{x}) |x\rangle |q(\vec{x})\rangle, \quad (8)$$

where $f(\vec{x})$ is such that $\int_{\mathcal{R}} d\vec{x} |f(\vec{x})|^2 = 1$ and $|q(\vec{x})\rangle$ is a parametrized state of the discrete degrees of freedom:

$$|q(\vec{x})\rangle = \sum_{s=0}^{d^M-1} \sqrt{p_s(\vec{x})} e^{i\phi_s(\vec{x})} |s\rangle,$$

where $\{p_s(\vec{x}), \phi_s(\vec{x})\}_s$ is a set of $2(d^M - 1)$ real functions such that $\sum_{s=0}^{d^M-1} p_s(\vec{x}) = 1$, $\phi_s(\vec{x}) \in [0, 2\pi]$, and $\{|s\rangle\}_{s=0}^{d^M-1}$ is a basis on \mathcal{H}_M^d .

(The Supplementary Material gives the proof.) Equation (8)'s state parametrization preserves key information about the continuous degrees of freedom, namely $|f(\vec{x})|^2$, when working with the discrete degrees of freedom. Indeed, the partial trace over the continuous degrees of freedom yields:

$$\rho = \int_{\mathcal{R}} d\vec{x} |f(\vec{x})|^2 |q(\vec{x})\rangle \langle q(\vec{x})|.$$

Continuing, given an observable \mathcal{O} with support only on

\mathcal{H}_M^d , we have:

$$\langle \mathcal{O} \rangle = \text{Tr } \rho \mathcal{O} = \int_{\mathcal{R}} d\vec{x} |f(\vec{x})|^2 \mathcal{O}(q(\vec{x})),$$

where $\mathcal{O}(q(\vec{x})) = \langle q(\vec{x}) | \mathcal{O} | q(\vec{x}) \rangle$. Comparing with Eq. (4) one realizes that the functions $\{p_s(\vec{x}), \phi_s(\vec{x})\}$ provide an \vec{x} -dependent embedding of $\mathcal{R} \subseteq \mathbb{R}^N$ onto $\mathbb{C}P^n$, with $n = d^M - 1$, or a submanifold, via:

$$\Phi : \vec{x} \rightarrow \Phi(\vec{x}) = Z(\vec{x}),$$

where:

$$Z = (Z^0, \dots, Z^n),$$

with $Z^\alpha(\vec{x}) = \sqrt{p_\alpha(\vec{x})} e^{i\phi_\alpha(\vec{x})}$. Thus, letting $\mathcal{R}^* = \Phi(\mathcal{R})$, we obtain:

$$\int_{\mathcal{R}} d\vec{x} |f(\vec{x})|^2 \mathcal{O}(q(\vec{x})) = \int_{\mathcal{R}^*} dV_{FS} q(Z) \mathcal{O}(Z),$$

where:

$$q(Z) = \frac{|\det D\Phi(Z)|}{\sqrt{\det g_{FS}}} |f(\Phi^{-1}(Z))|^2.$$

Here, $D\Phi$ denotes the Jacobian of the transformation Φ and g_{FS} is the Fubini-Study metric tensor and we assume the transformation is invertible. Generalizing to cases in which Φ^{-1} is not invertible, due to the fact that different \vec{x} might yield the same $(p_s(\vec{x}), \phi_s(\vec{x}))$, is left to future efforts.

Let's illustrate with a familiar system: an electron in a 2D rectangular box $\mathcal{R} = [x_0, x_1] \times [y_0, y_1]$. In this case, $M = 1$ and $d = 2$ so that we have $f(x, y), \{p_s(x, y), \phi_s(x, y)\}_{s=0,1}$. This amounts to:

$$\begin{aligned} & \int_{x_0}^{x_1} dx \int_{y_0}^{y_1} dy |f(x, y)|^2 \mathcal{O}(q(x, y)) \\ &= \frac{1}{2} \int_0^1 dp \int_0^{2\pi} d\phi q(Z(p, \phi)) \mathcal{O}(Z(p, \phi)), \end{aligned}$$

where, for example, $p_0(x, y) = 1 - p_1(x, y)$, $p_1(x, y) = \frac{x-x_0}{x_1-x_0}$, $\phi_0(x, y) = 0$, and $\phi_1(x, y) = 2\pi \frac{y-y_0}{y_1-y_0}$.

In short, a generic quantum state $|\psi\rangle$ of the whole system uniquely defines a distribution $q(Z)$ on the manifold of pure states $\mathcal{P}(\mathcal{H}_M^d) = \mathbb{C}P^{d^M-1}$. The correspondence is not one-to-one as knowledge of $q(Z)$ does not allow recovering the entire state. The missing part is $\theta_0(\vec{x})$, the phase of $f(\vec{x})$. However, it does circumscribe the possible states as it fixes the shape of the probability distribution of the continuous variables $|f(\vec{x})|^2$.

Note how the embedding functions $p_s(\vec{x})$ and $\phi_s(\vec{x})$ play a key role in determining whether we can cover the whole $\mathbb{C}P^n$ or just a submanifold. Consider the conditions that guarantee the two extreme cases are covered: full covering of $\mathbb{C}P^n$ and covering of tensor product states only $\mathbb{C}P^{d-1} \otimes \dots \otimes \mathbb{C}P^{d-1}$. In the first case, $\mathbb{C}P^n$ is

a complex manifold that requires $2n$ independent real coordinates to be completely covered. For M qudits this means:

$$\begin{aligned} M &\leq M_{\max}^{\text{Full}} \\ &= \frac{\log(N/2 + 1)}{\log d} . \end{aligned}$$

Instead, if we need to cover only the submanifold of tensor product states, the number of qudits we can control with N continuous degrees of freedom is much larger:

$$\begin{aligned} M &\leq M_{\max}^{\text{Prod}} \\ &= \frac{N}{2(d-1)} . \end{aligned}$$

Most cases fall in between. And so, the number of qudits controllable with N continuous variables is $M \in [M_{\max}^{\text{Full}}, M_{\max}^{\text{Prod}}]$.

Thermodynamic framework. Another setting in which the geometric formalism arises naturally is quantum thermodynamics. There, one is often interested in modeling the behavior of a small system in a thermal environment. For modest-sized environments one can naively treat the system and environment as isolated and then simulate its evolution. As the environment's size grows, this quickly becomes infeasible. Nonetheless, as we now show, the geometric formalism allows appropriately writing the system's reduced density matrix in a way that retains much of the information about the environment. This can be done due to Thm. 1.

Consider a large quantum system consisting of M qudits split in two asymmetric parts. Call the small part with N_S qudits the "system" and let the rest be the "environment" with $N_E = M - N_S$ qudits. A generic state of the entire system $\mathcal{H}_S \otimes \mathcal{H}_E$ is $|\psi_{SE}\rangle = \sum_{k=0}^{d_S-1} \sum_{\alpha=0}^{d_E-1} \psi_{k\alpha} |s_k\rangle |e_\alpha\rangle$, where $\{|s_k\rangle\}_k$ and $\{|e_\alpha\rangle\}_\alpha$ are bases for \mathcal{H}_S and \mathcal{H}_E , respectively.

Given $|\psi_{SE}\rangle$, it is not too hard to see that the system's (reduced) state is:

$$\rho^S = \sum_{\alpha=1}^{d_E} p_\alpha^S |\chi_\alpha^S\rangle \langle \chi_\alpha^S| , \quad (9)$$

where:

$$p_\alpha^S = \sum_{k=0}^{d_S-1} |\psi_{k\alpha}|^2 ,$$

and

$$|\chi_\alpha^S\rangle = \frac{1}{\sqrt{p_\alpha^S}} \sum_{k=0}^{d_S-1} \psi_{k\alpha} |s_k\rangle .$$

In numerical analysis one often retains only the $d_S \times d_S$ matrix elements of ρ^S in a certain basis. However, this

erases the functional information about the environment. Instead, the latter can be recovered from $\{p_\alpha^S, |\chi_\alpha^S\rangle\}$ as:

$$(\rho^E)_{\alpha\beta} = \sqrt{p_\alpha^S p_\beta^S} \langle \chi_\alpha^S | \chi_\beta^S \rangle .$$

As d_E grows, retaining this information as a set of probabilities and states quickly becomes unrealistic.

However, the same information can be effectively encoded by switching to a geometric description. Indeed, at finite d_E , ρ^S becomes:

$$p_{d_E}^S(Z) = \sum_{\alpha=1}^{d_E} p_\alpha^E \tilde{\delta} [Z - Z(\chi_\alpha^S)]$$

and the thermodynamic limit is conveniently handled with:

$$p_\infty(Z) = \lim_{d_E \rightarrow \infty} \sum_{\alpha=1}^{d_E} p_\alpha^E \tilde{\delta} [Z - Z(\chi_\alpha^S)] .$$

Here the limit is performed, as usual, by keeping finite the average energy density $\lim_{d_E \rightarrow \infty} \langle H \rangle / (N_S + N_E) = \epsilon$.

In this way, the geometric formalism emerges naturally in a quantum thermodynamics. In the limit of large environments, one simply cannot keep track of exactly how an environment generates the ensemble of our system under study and so switch to a probabilistic description. Helpfully, the geometric formalism efficiently controls this. See also Ref. [5] for an expanded exploration of the geometric formalism in quantum thermodynamics.

Before proceeding, though, let's highlight an interesting discrepancy between the two applications presented. In the thermodynamic setting, knowledge of the ensemble $\{p_\alpha^S, |\chi_\alpha^S\rangle\}$ allows fully recovering the global pure state $|\psi_{SE}\rangle$. Indeed, it is easy to see that:

$$\psi_{k\alpha} = \sqrt{p_\alpha^S} \langle s_k | \chi_\alpha^S \rangle .$$

Substituting this into the pure state $|\psi_{SE}\rangle$, we obtain a Schmidt-like decomposition in which the common label runs over the dimension of the environment's Hilbert space:

$$|\psi_{SE}\rangle = \sum_{\alpha=0}^{d_E-1} \sqrt{p_\alpha^S} |\chi_\alpha^S\rangle |e_\alpha\rangle .$$

The price paid for the decomposition is that the states $|\chi_\alpha^S\rangle$ are not orthogonal. However, we gain a more detailed description of our system's state. As we can see, here the challenge of recovering $|\psi_{SE}\rangle$ disappears thanks to $p_\alpha^S \in \mathbb{R}$. We comment on this discrepancy with the other case shortly.

Discussion. Standard quantum mechanics' concept of state is the density matrix. However, while density matrices provide a complete account of POVM statistics, they are not in one-to-one correspondence with the en-

sembles that generated them. This is a well-known fact that underlies the freedom in writing a decomposition of the density matrix in terms of probabilities and pure states. All such decompositions yield the same POVM statistics, but they are not physically equivalent since they are realized in physically different ways.

From a purification perspective [28], the physical information about an ensemble’s realization can always be thought of as coming from a larger system that is in a pure state. While the additional information about how the ensemble is realized is not relevant for the measurement statistics on our system, it does provide a much richer description. It preserves part (if not all) of the structural information about how the system’s POVM statistics result from interactions with its surroundings.

Geometric quantum mechanics and its concept of geometric quantum state provide a framework that allows retaining such information. This yields a richer picture of the system’s state which goes beyond the system’s POVM statistics, taking into account the physical way in which an ensemble has been realized. The geometric formalism’s benefits emerge in at least two important cases: (i) Hybrid continuous-discrete systems, e.g., electrons or other particles with spin or other discrete degrees of freedom, and (ii) the thermodynamic setting of a system in contact with a large environment.

The geometric formalism directly handles the continuous nature of hybrid systems and the large number of degrees of freedom in thermodynamics. And, it does so in a fairly simple way. This allows working with the full geometric quantum state, thus retaining the structural information about how the ensemble is generated. While the two applications considered are similar, a crucial difference does appear. If we assume a finite environment, knowledge of the geometric quantum state of our system is sufficient to recover the global pure state of system and environment. This does not occur for a hybrid discrete-continuous system, where knowledge of the geometric quantum state does not allow inferring the phase $\theta_0(\vec{x})$ of $f(\vec{x})$. Notably, fully recovering the overall pure state, whose physical relevance can be argued on the ground of continuity with the finite-dimensional case, effectively translates into a $U(1)$ gauge principle on the overall system. The requirement that states differing from a local phase are physically equivalent— $\psi_s(\vec{x}) \sim e^{i\varphi(\vec{x})}\psi_s(\vec{x})$ —turns into a sufficient condition for recovering the global state from the geometric quantum state since, in this case,

one can always choose $f(\vec{x}) \in \mathbb{R}$. We leave exploring the connection between recovering the global pure state from a local geometric quantum state and a gauge principle for a future investigation.

Conclusion. Geometric quantum mechanics is an alternative to the standard vector-based formalism. We introduced and then explored the concept of *geometric quantum state* $p(Z)$ as a probability distribution on the manifold of pure states, inspired by the statistics of chaotic attractors from the theory of dynamical systems or, more appropriately, its Sinai-Bowen-Ruelle measures [1]. This characterization of a quantum state accounts for the fact that singling out the density matrix as the sole descriptor of a quantum system’s state entails ignoring how an ensemble is physically realized. While this does not have consequences for POVM statistics, in concrete situations the information about the ensemble realization can be key to accurate modeling. Reference [4] gives an example. That said, density matrices can be readily computed as quadratic averages from $p(Z)$ via Eq. (7).

We explored the physical relevance of geometric quantum states via an open quantum system in which a (finite) system under study is in contact with a larger environment and the joint state is assumed to be pure. In this thermodynamic setting, portions of the structural information about the joint pure state is directly preserved in the geometric quantum state of the smaller system under study. The result is a markedly richer picture of the system’s state—a picture that goes substantially beyond the density matrix and its POVM statistics.

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 Dhurva Karkada for his help with the example, David Gier, 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.

-
- [1] J. Eckmann and D. Ruelle. Ergodic theory of chaos and strange attractors. *Rev. Mod. Phys.*, 57:617–656, 1985.
 - [2] R. K. Pathria and Paul D. Beale. *Statistical Mechanics*. Elsevier B.V., 2011.
 - [3] W. Greiner, L. Neise, and H. Stöcker. *Thermodynamics and Statistical Mechanics*. Springer New York, New York, NY, 1995.
 - [4] F. Anza and J. P. Crutchfield. Geometric quantum state estimation. *in preparation*, 2020.
 - [5] F. Anza and J. P. Crutchfield. Geometric quantum thermodynamics. *in preparation*, 2020.
 - [6] F. Strocchi. Complex Coordinates and Quantum Mechanics. *Rev. Mod. Phys.*, 38(1):36–40, 1966.

- [7] T. W. B. Kibble. Geometrization of quantum mechanics. *Comm. Math. Physics*, 65(2):189–201, 1979.
- [8] André Heslot. Quantum mechanics as a classical theory. *Phys. Rev. D*, 31(6):1341–1348, 1985.
- [9] G. W. Gibbons. Typical states and density matrices. *J. Geom. Physics*, 8(1-4):147–162, 1992.
- [10] A. Ashtekar and T. A. Schilling. Geometry of quantum mechanics. In *AIP Conference Proceedings*, volume 342, pages 471–478. AIP, 1995.
- [11] 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.
- [12] D. C. Brody and L. P. Hughston. Geometric quantum mechanics. *J. Geom. Physics*, 38(1):19–53, 2001.
- [13] I. Bengtsson and K. Życzkowski. *Geometry of Quantum States*. Cambridge University Press, Cambridge, 2017.
- [14] J. F. Cariñena, J. Clemente-Gallardo, and G. Marmo. Geometrization of quantum mechanics. *Theo. Math. Physics*, 152(1):894–903, jul 2007.
- [15] D. Chruściński. Geometric Aspects of Quantum Mechanics and Quantum Entanglement. *J. Physics: Conf. Ser.*, 30:9–16, 2006.
- [16] G. Marmo and G. F. Volkert. Geometrical description of quantum mechanics—transformations and dynamics. *Physica Scripta*, 82(3):038117, 2010.
- [17] J. Avron and O. Kenneth. An elementary introduction to the geometry of quantum states with pictures. *Rev. Math. Physics*, 32(02):2030001, 2020.
- [18] D. Pastorello. A geometric Hamiltonian description of composite quantum systems and quantum entanglement. *Intl. J. Geo. Meth. Mod. Physics*, 12(07):1550069, 2015.
- [19] D. Pastorello. Geometric Hamiltonian formulation of quantum mechanics in complex projective spaces. *Intl. J. Geom. Meth. Mod. Physics*, 12(08):1560015, 2015.
- [20] D. Pastorello. Geometric Hamiltonian quantum mechanics and applications. *Intl. J. Geo. Meth. Mod. Physics*, 13(Supp. 1):1630017, 2016.
- [21] J. Clemente-Gallardo and G. Marmo. The Ehrenfest picture and the geometry of Quantum Mechanics. *Il Nuovo Cimento C*, 3:35–52, 2013.
- [22] M. A. Nielsen and I. L. Chuang. *Quantum computation and quantum information*. Cambridge University Press, 2010.
- [23] T. Heinosaari and M. Ziman. *The mathematical language of quantum theory*. Cambridge University Press, 2012.
- [24] F. Strocchi. *An introduction to the mathematical structure of quantum mechanics: A short course for mathematicians*. World Scientific, 2008.
- [25] D. C. Brody and L. P. Hughston. The quantum canonical ensemble. *J. Math. Physics*, 39(12):6502–6508, 1998.
- [26] D. C. Brody and L. P. Hughston. Thermodynamics of quantum heat bath. *J. Physics A: Math. Theo.*, 49(42):425302, 2016.
- [27] M. Pasini, N. Leone, S. Mazzucchi, V. Moretti, D. Pastorello, and L. Pavesi. Bell inequality violation by entangled single photon states generated from a laser, a LED or a Halogen lamp. *arXiv:2003.09961*, 2020.
- [28] M. M. Wilde. *Quantum Information Theory*. Cambridge University Press, Cambridge, 2017.
- [29] L. de Broglie. Recherches sur la théorie des quanta. *Ann. de Physique*, 3(10):22, 1925.
- [30] E. Schrodinger. An undulatory theory of the mechanics of atoms and molecules. *Phys. Rev.*, 28(6):1049–1070, 1926.
- [31] J. v. Neumann. Thermodynamik quantummechanischer gesamtheiten. *J. Gottingr Nachr.*, 1:245,273, 1927.
- [32] J. v. Neumann. *Mathematische Grundlagen der Quantenmechanik*. Springer-Verlag, 1932.
- [33] P. A. M. Dirac. The basis of statistical quantum mechanics. *Math. Proc. Camb. Phil. Soc.*, 25(1):62–66, 1929.
- [34] P. A. M. Dirac. Note on exchange phenomena in the Thomas atom. *Math. Proc. Camb. Phil. Soc.*, 26:376, 1930.
- [35] P. A. M. Dirac. Note on the interpretation of the density matrix in the many-electron problem. *Math. Proc. Camb. Phil. Soc.*, 27(2):240–243, 1931.
- [36] W. Heisenberg. über quantentheoretische umdeutung kinematischer und mechanischer beziehungen. *Zeit. für Physik*, 33:879–893, 1925.

Supplementary Materials

Beyond Density Matrices: Geometric Quantum States

Fabio Anza and James P. Crutchfield

Appendix A: The Search for Quantum States

In those domains of the physical sciences that concern the organization and evolution of systems, a common first task is to determine a system's distinct configurations or *effective states*. Ultimately, this turns on what questions there are to answer. One goal is prediction—of properties or behaviors. And, in this, quantum mechanics stands out as a particularly telling arena in which to define effective states.

The very early history of its development can be construed partially as attempts to answer this question, from de Broglie's *phase-waves* [29] and Schrodinger's *wave functions* [30] to von Neumann's *statistical operators* in Refs. [31] and [32, Chap. IV], later labeled *density matrices* by Dirac [33–35]. And, these were paralleled by Heisenberg's “operational” *matrix mechanics* that focused on experimentally accessible observables and so avoided imputing internal, hidden structure [36].

The abiding challenge is that effective states are almost always inferred indirectly and through much trial and error. Quantum mechanics heightens the challenge greatly due to its foundational axiom that the detailed, microscopic, and fundamental degrees of freedom cannot be directly and completely measured *in principle*. The main text revisits this perennial question, What is a quantum state?

Appendix B: Theorem 1: Proof

In this Appendix we give the detailed proof of Theorem 1 in the main text. Let's first restate the setup of the theorem. Consider a hybrid quantum system comprised of N continuous degrees of freedom and M qudits that are the discrete ones. The entire system's Hilbert space is:

$$\mathcal{H} = \mathcal{H}_N^c \otimes \mathcal{H}_M^d ,$$

where \mathcal{H}_N^c hosts the continuous degrees of freedom and has infinite dimension, while \mathcal{H}_M^d hosts the discrete ones and has dimension d^M . A basis for \mathcal{H}_N^c is provided by $\{|\vec{x}\rangle\}$, where $\vec{x} \in \mathcal{R} \subseteq \mathbb{R}^N$ and a basis for \mathcal{H}_M^d is $\{|s\rangle\}_{s=0}^{d^M-1}$. Thus, a generic state is:

$$|\psi\rangle = \int_{\mathcal{R}} d\vec{x} \sum_s \psi_s(\vec{x}) |\vec{x}\rangle |s\rangle ,$$

where \vec{x} is a dimensionless counterpart of the physical continuous degrees of freedom, achieved by multiplying its value by appropriate physical quantities. So, the measure $d\vec{x}$ has no physical dimension.

Theorem 1. *Any state $|\psi\rangle \in \mathcal{H}$ can be written as:*

$$|\psi\rangle = \int_{\mathcal{R}} d\vec{x} f(\vec{x}) |x\rangle |q(\vec{x})\rangle ,$$

where $f(\vec{x})$ is such that $\int_{\mathcal{R}} d\vec{x} |f(\vec{x})|^2 = 1$ and $|q(\vec{x})\rangle$ is a parametrized state of the discrete degrees of freedom:

$$|q(\vec{x})\rangle = \sum_{s=0}^{d^M-1} \sqrt{p_s(\vec{x})} e^{i\phi_s(\vec{x})} |s\rangle ,$$

where $\{p_s(\vec{x}), \phi_s(\vec{x})\}_s$ is a set of $2(d^M - 1)$ real functions such that $\sum_{s=0}^{d^M-1} p_s(\vec{x}) = 1$, $\phi_s(\vec{x}) \in [0, 2\pi]$, and $\{|s\rangle\}_{s=0}^{d^M-1}$ is a basis for \mathcal{H}_M^d .

Proof: The proof is constructive. Given an arbitrary $\{\psi_s(\vec{x})\}_s$, we can always find the set of functions $f(\vec{x})$, $p_s(\vec{x})$, and $\phi_s(\vec{x})$. The converse holds trivially: Given these functions one can always compute the $\{\psi_s(\vec{x})\}_s$. The set of

transformations that maps one parametrization into the other is:

$$\phi_s(\vec{x}) = \theta_s(\vec{x}) - \theta_0(\vec{x}) ,$$

where:

$$e^{i\theta_s(\vec{x})} = \frac{\psi_s(\vec{x})}{|\psi_s(\vec{x})|} .$$

Moreover:

$$f(\vec{x}) = \sqrt{\sum_{s=0}^{d^M-1} |\psi_s(\vec{x})|^2} e^{i\theta_0(\vec{x})} \text{ and}$$

$$p_s(\vec{x}) := \frac{|\psi_s(\vec{x})|^2}{\sum_{l=0}^{d^M-1} |\psi_l(\vec{x})|^2} ,$$

It is easy to see how normalization of $|f(\vec{x})|^2$ and of $p_s(\vec{x})$ emerges from the definitions:

$$\begin{aligned} \int_{\mathcal{R}} d\vec{x} |f(\vec{x})|^2 &= \int_{\mathcal{R}} d\vec{x} \sum_{s=0}^{d^M-1} |\psi_s(\vec{x})|^2 \\ &= 1 , \\ \sum_{s=0}^{d^M-1} p_s(\vec{x}) &= \sum_{s=0}^{d^M-1} \frac{|\psi_s(\vec{x})|^2}{\sum_{l=0}^{d^M-1} |\psi_l(\vec{x})|^2} \\ &= 1 , \text{ and} \\ |e^{i\phi_s(\vec{x})}|^2 &= \frac{|\psi_s(\vec{x})|}{|\psi_s(\vec{x})|} \\ &= 1 . \end{aligned}$$

The latter gives $\phi_s(\vec{x}) \in [0, 2\pi]$.

With these definitions we obtain:

$$\begin{aligned} e^{i\phi_s(\vec{x})} f(\vec{x}) \sqrt{p_s(\vec{x})} &= \sqrt{|\psi_s(\vec{x})|^2} e^{i\theta_s(\vec{x})} \\ &= \psi_s(\vec{x}) . \end{aligned}$$

This in turn gives the desired result:

$$\begin{aligned} |\psi\rangle &= \int_{\mathcal{R}} d\vec{x} \sum_s \psi_s(\vec{x}) |\vec{x}\rangle |s\rangle \\ &= \int_{\mathcal{R}} d\vec{x} f(\vec{x}) |\vec{x}\rangle \sum_s e^{i\phi_s(\vec{x})} \sqrt{p_s(\vec{x})} |s\rangle \\ &= \int_{\mathcal{R}} d\vec{x} f(\vec{x}) |x\rangle |q(\vec{x})\rangle . \end{aligned}$$