

* fanza@ucdavis.edu

operator \mathcal{O} on state $|\psi\rangle$ with coordinates Z :

$$\mathcal{O}(Z) = \frac{\sum_{\alpha,\beta} \mathcal{O}_{\alpha,\beta} Z^\alpha \bar{Z}^\beta}{\sum_\gamma |Z^\gamma|^2}, \quad (1)$$

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 $|\psi\rangle$. 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:

$$E_j(Z) = \frac{\sum_{\alpha,\beta} (E_j)_{\alpha,\beta} Z^\alpha \bar{Z}^\beta}{\sum_\gamma |Z^\gamma|^2}, \quad (2)$$

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

The quantum state space $\mathcal{P}(\mathcal{H})$ has a preferred metric g_{FS} —the *Fubini-Study metric* [?]—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 $Z^\alpha = \sqrt{p_\alpha} e^{i\phi_\alpha}$ 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 $\nu_0 = 0$. As we will see now, these coordinates play a particular role: they are canonically conjugated.

State-space structure. Beyond the Riemannian structures, it can be shown that $\mathcal{P}(\mathcal{H})$ also has another interesting geometric feature: a symplectic structure. This is the hallmark of classical state spaces and justifies the use of the term *quantum state space* for $\mathcal{P}(\mathcal{H})$. With a more common jargon, a symplectic structure is the geometric entity allowing us to define ‘‘Poisson Brackets’’ and the existence of canonically conjugated coordinates. In particular, using probabilities and phases coordinates $\{(p_\alpha, \phi_\alpha)\}$ one has that $\{p_\alpha, \phi_\beta\} = \frac{1}{\hbar} \delta_{\alpha\beta}$. Thus, for arbitrary functions A and B on $\mathcal{P}(\mathcal{H})$ one has

$$\{A, B\} := \frac{1}{\hbar} \sum_{\alpha=1}^{D-1} \frac{\partial A}{\partial p_\alpha} \frac{\partial B}{\partial \phi_\alpha} - \frac{\partial B}{\partial p_\alpha} \frac{\partial A}{\partial \phi_\alpha} \quad (3)$$

Unitary evolution. In QM, an isolated quantum system evolves with a unitary propagator $U(t, t_0) = e^{-\frac{i}{\hbar} H(t-t_0)}$,

where the generator H is the (time-independent) Hamiltonian of the system. Surprisingly, it can be shown [?] that this evolution is equivalent to a classical Hamiltonian dynamics, with geometric coordinates. In particular, calling $E(p_\alpha, \phi_\alpha) = \langle \psi(p_\alpha, \phi_\alpha) | H | \psi(p_\alpha, \phi_\alpha) \rangle$ the expectation value of H on a generic state $|\psi(p_\alpha, \phi_\alpha)\rangle = \sum_{\alpha=0}^{D-1} \sqrt{p_\alpha} e^{i\phi_\alpha} |e_\alpha\rangle$ parametrized by (p_α, ϕ_α) , the unitary of a generic function A on $\mathcal{P}(\mathcal{H})$ is given by

$$\frac{\partial A}{\partial t} = \{A, E\} \quad (4)$$

Or, equivalently, a generic state $\{(p_\alpha, \phi_\alpha)\}$ evolves according to Hamilton's equations of motion:

$$\begin{aligned} \frac{dp_\alpha}{dt} &= \frac{1}{\hbar} \frac{\partial E}{\partial \phi_\alpha} \\ \frac{d\phi_\alpha}{dt} &= -\frac{1}{\hbar} \frac{\partial E}{\partial p_\alpha} \end{aligned}$$

Here the analogies with classical Hamiltonian mechanics are particularly evident. While quantum mechanics is clearly very different from its classical counterpart, at a certain descriptive level we can still use the intuition of classical mechanics to understand the unitary evolution of quantum systems. Thus, as we do for classical mechanics and statistical physics, we continue by introducing probability distributions on the quantum state space.

Geometric quantum states. The geometric framework makes it very natural to view a quantum state as a functional encoding that associates expectation values to observables, paralleling the C^* -algebra formulation of quantum mechanics [?]. The idea is that one considers probability density functions on $\mathcal{P}(\mathcal{H})$ (as $q(Z)$), together with observable functions (as $\mathcal{O}(Z)$). This was introduced in Ref. [?] and here we give a quick summary.

States are functionals $P[\mathcal{O}]$ from the algebra of observables \mathcal{A} to the real line:

$$P_q[\mathcal{O}] = \int_{\mathcal{P}(\mathcal{H})} q(Z) \mathcal{O}(Z) dV_{FS}, \quad (5)$$

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, kets $|\psi_0\rangle$ 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 coordi-

nates this reads:

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

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

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

where the coordinate-invariant nature of the functionals $P_q[\mathcal{O}]$ is now apparent. Extending by linearity, 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 tools, one identifies the distribution $q(Z)$ of Eq. (5) as a system's *geometric quantum state*. This is a generalized notion of quantum state.

A simple example of a geometric quantum 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 was introduced in Refs. [?]. References [?] and [?] 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.

Density matrix. The connection between geometric quantum states and density matrices is two-fold. On the one hand, when $q(Z)$ 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 than density matrices.

On the other hand, given an arbitrary $q(Z)$, 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 to the specific form of POVMs on $\mathcal{P}(\mathcal{H})$, recall Eq. (2), they are sensitive to $q(Z)$ only via ρ^q . Therefore, if two geometric quantum states 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 physical configurations are the same. 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:

$$q_1(Z) = 0.864 \tilde{\delta}(Z - Z_+) + 0.136 \tilde{\delta}(Z - Z_-) ,$$

$$q_2(Z) = \frac{1}{Q} e^{-\frac{1}{2} \bar{Z} \rho^{-1} Z} ,$$

where $Q = \int_{\mathbb{C}P^1} dV_{FS} e^{-\frac{1}{2} \bar{Z} \rho^{-1} Z}$, $Z_+ = (0.657, 0.418 + i0.627)$, 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.

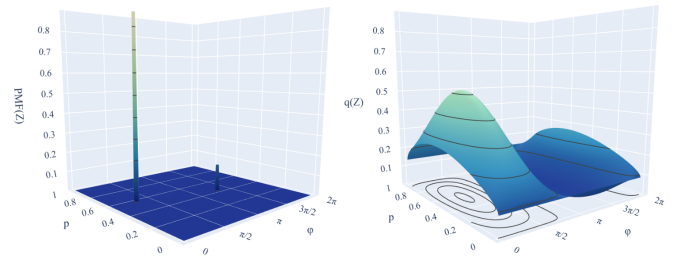


Figure 1. Geometric quantum states in $(probability, phase)$ coordinates (p, ϕ) of $\mathbb{C}P^1$: (Left) Geometric quantum state q_1 is the convex sum of two Dirac delta-functions, centered on the eigenvectors $(p_+, \phi_+) = (0.568, 0.983)$ and $(p_-, \phi_-) = (0.432, 4.124)$ of density matrix ρ . (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 $\rho_- = 0.136$. Thus, the marked difference in the structure of geometric quantum states q_1 and q_2 is not reflected in their shared density-matrix $\rho_1 = \rho_2 = \rho$.

II. INFORMATION TRANSPORT

III. DYNAMICS

IV. EXAMPLES

V. CONCLUSIONS

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 ensembles 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. The abiding question then becomes: Which of these physically different ways exhibit observable or, even perhaps, manipulable phenomena?

From a purification perspective [?], 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 description of the system—one that goes beyond the system's POVM statistics, taking into account the physical manner 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 direct way. Thus, the geometric quantum state retains the structural information about how an ensemble is generated. While the two applications considered are similar, a crucial difference appears.

If we assume a finite environment, knowledge of the geometric quantum state of our system is sufficient to recover the globally pure joint 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 wave-functions 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 pure state from the local geometric quantum state since, in this case, one can always choose $f(\vec{x}) \in \mathbb{R}$. Effectively, this is the principle behind gauge symmetries and gauge theories. We must 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 thermodynamic formalism of chaotic attractors from the theory of dynamical systems or, more appropriately, its Sinai-Bowen-Ruelle measures [?]. This characterization 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 observable consequences if one is restricted to POVM statistics, in concrete situations the information about the ensemble realization can be key to accurate modeling. Reference [?] gives an example. That said, the geometric setting is always sufficiently general that density matrices are 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 their 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.

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Supplementary Materials

A kinetic theory of quantum information

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* [?] and Schrodinger's *wave functions* [?] to von Neumann's *statistical operators* in Refs. [?] and [?, Chap. IV], later labeled *density matrices* by Dirac [? ? ?]. And, these were paralleled by Heisenberg's “operational” *matrix mechanics* that focused on experimentally accessible observables and so avoided imputing internal, hidden structure [?].

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 ??: Proof

This Appendix gives proves in detail Theorem ??. Let's first restate its setup.

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:

$$|\psi\rangle = \int_{\mathcal{R}} d\vec{x} \sum_s \psi_s(\vec{x}) |\vec{x}\rangle |s\rangle , \quad (\text{B1})$$

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 ??. *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 $\{\psi_s(\vec{x})\}_s$. First, we define

$\theta_s(\vec{x})$ as the phase of $\psi_s(\vec{x})$:

$$\theta_s(\vec{x}) \in [0, 2\pi[\quad \text{such that} \quad \psi_s(\vec{x}) = |\psi_s(\vec{x})| e^{i\theta_s(\vec{x})} ,$$

and define the functions

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

Starting from Eq.(B1) this gives

$$\begin{aligned} |\psi\rangle &= \int_{\mathcal{R}} d\vec{x} \sum_s \psi_s(\vec{x}) |\vec{x}\rangle |s\rangle = \int_{\mathcal{R}} d\vec{x} \sum_s |\psi_s(\vec{x})| e^{i\theta_s(\vec{x})} |\vec{x}\rangle |s\rangle = \int_{\mathcal{R}} d\vec{x} \sum_s |\psi_s(\vec{x})| e^{i\phi_s(\vec{x}) + i\theta_0(\vec{x})} |\vec{x}\rangle |s\rangle \\ &= \int_{\mathcal{R}} d\vec{x} e^{i\theta_0(\vec{x})} \sum_s |\psi_s(\vec{x})| e^{i\phi_s(\vec{x})} |\vec{x}\rangle |s\rangle \end{aligned}$$

We now define $f(\vec{x})$ and $p_s(\vec{x})$ as follows:

$$\begin{aligned} f(\vec{x}) &:= \sqrt{\sum_{s=0}^{d^M-1} |\psi_s(\vec{x})|^2} e^{i\theta_0(\vec{x})} \text{ and} \\ p_s(\vec{x}) &:= \frac{|\psi_s(\vec{x})|^2}{\sum_{l=0}^{d^M-1} |\psi_l(\vec{x})|^2} , \end{aligned}$$

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:

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