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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

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A quantum system's state is often 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 the physical realization of an ensemble. Fortunately, when working only with the statistical outcomes of positive-operator values measurements (POVMs) this is not a hindrance. Here we explore the notion of geometric quantum state, as a way to keep track of the ensemble realization, and its physical relevance. We emphasize two main perspectives: quantum control and quantum thermodynamics. **HERE** Its geometric quantum states are complete and, if needed, the density matrix description can be extracted from them.

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Quantum mechanics is firmly rooted in a vector formalism where a system's 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. One transforms states in $\mathcal{H}$ using density matrices ρ, operators that are positive semi-definite $\rho \geq 0$, self-adjoint $\rho = \rho^\dagger$, and normalized $\mathrm{Tr}\,\rho = 1$. The interpretation of a density matrix as a system's *probabilistic state* is given by *ensemble theory* [1, 2]. Accordingly, since a density matrix always decomposes into eigenvalues λ_i and eigenvectors $|\lambda_i\rangle$:

$$\rho = \sum_i \lambda_i \, |\lambda_i\rangle \, \langle\lambda_i| \ ,$$

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

However, this interpretation is problematic: It is not unique. One can write the same ρ using different decompositions:

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

that, nonetheless, all identify the same quantum state. While one often prefers the diagonal decomposition in terms of eigenvalues and eigenvectors, this is not the only possible decomposition. More tellingly, in principle, there is no experimental reason to prefer it to other decompositions. 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 has an infinite number of identical decompositions, each possibly being a distinct ensemble.

JPC: Need a short definition of mixed state above so that maximally-mixed makes at least intuitive understanding here in the Introduction.

Moreover, it is rather straightforward to imagine systems that, despite having the same density matrix, are in a different state. 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 case, always prepare states $\{|-\rangle, |+\rangle\}$ each with probability 1/2. A complete and unambiguous mathematical characterization of the notion of state should not conflate these distinct physical configurations.

So, here we argue that the geometric formalism, together with an appropriately formulated measure theory, allows to separate between the primary notion of *state of the system* and the derived notion of density matrix as the set of all *POVM statistics* on that system.

With this perspective in mind, we introduce a more incisive description of pure-state ensembles. The following argues that *geometric quantum mechanics* (GQM), with its notion of *geometric quantum states*, cleanly resolves the ambiguities. First, we introduce GQM. Second, we discuss how it relates to the more familiar density matrix formalism and how it handles outcomes of quantum measurements. Third, **WHAT?**.

Geometric quantum mechanics. References [3–18] 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 $\mathcal{P}(\mathcal{H}) = \mathbb{C}\mathrm{P}^{D-1}$. 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, we have

$Z = (\sqrt{p_0}e^{i\nu_0}, \sqrt{p_1}e^{i\nu_1})$.

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

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

with $\mathcal{O}_{\beta,\alpha} = \overline{\mathcal{O}}_{\alpha,\beta}$.

The probabilities of measurement outcomes are given by *positive operator-valued measurements* (POVMs) $\{E_j\}_{j=1}^n$. 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 are a collection of nonnegative real functions $E_j(Z) \geq 0$ on $\mathcal{P}(\mathcal{H})$ whose sum is always equal to one:

$$E_j(Z) = \sum_{\alpha,\beta} (E_j)_{\alpha,\beta} Z^\alpha \overline{Z}^\beta \ , \tag{2}$$

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* [10]—and an associated volume element that is coordinate-independent and invariant under unitary changes. This is the Fubini-Study volume element, which we denote dV_{FS}. 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 + phases" coordinate system ($Z^\alpha = \sqrt{p_\alpha}e^{i\nu_\alpha}$) that we will use for concrete calculations:

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

Notice, here, 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, as done in the C^*-algebras formulation of quantum mechanics [19]. Thus, states can be described via functionals $P[\mathcal{O}]$ from the algebra of observables $\mathcal{A}$ to the real line:

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

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

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

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

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

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

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

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

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

$$\widetilde{\delta}(Z - Z_0) = \prod_{\alpha=1}^{D-1} 2\delta(p_\alpha - p_\alpha^0)\delta(\nu_\alpha - \nu_\alpha^0) \ , \tag{3}$$

where the coordinate-invariant nature of the functionals $P_p[\mathcal{O}]$ 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-like functionals:

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

Thus, the mixed states expressed as functionals from observables to the real line are:

$$P_{\text{mix}}\,[\mathcal{O}] = \sum_j \lambda_j \,\langle\lambda_j|\,\mathcal{O}\,|\lambda_j\rangle \ . \tag{4}$$

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

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

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

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. [20, 21]. Reference [**?**] 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 was shown in Ref.[**?**] that such ensemble is genuinely different from Gibbs ensemble, providing an experimental venue to test the experimental relevance of the geometric quantum state.

Density matrix. The connection between geometric quantum states and density matrices is two-fold. On the one hand, when the distribution $p(Z)$ 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 are of these simple Dirac-delta-like form. Thus, $p(Z)$ is clearly a more general notion of state of a quantum system.

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

$$\begin{aligned} \rho^p_{\alpha\beta} &= P_p[Z^\alpha \overline{Z}^\beta] \\ &= \int_{\mathcal{P}(\mathcal{H})} dV_{FS} \, p(Z) \, Z^\alpha \overline{Z}^\beta \ . \end{aligned} \tag{5}$$

Owing it to the fact that all POVMs are represented by real and quadratic functions on $\mathcal{P}(\mathcal{H})$, recall Eq. (2), they are not directly sensitive to $p(Z)$, but only to ρ^p. Therefore, if two distributions p_1 and p_2 induce the same density matrix $\rho^{p_1} = \rho^{p_2}$, 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. While this statement means that without further processing there is no POVM on the system that can distinguish between p_1 and p_2, it does not mean that there is no possible observable difference, as we explicitly demonstrate in the following.

We believe that this is particularly important for information processing tasks—as encountered in quantum computing, for example—in which one is not only interested in measurement outcomes, but also in understanding, predicting, and controlling how a quantum system responds to external manipulations. For the same reason, this formalism appears to emerge naturally in a quantum thermodynamics context, as argued in Ref.[**?**].

Distinguishability. Conventionally, two density matrices with the same barycenter are effectively equal. Due to this, one cannot distinguish two different physical configurations described by density matrices with the same barycenter. On the flip side, a given density matrix decomposes into distinct pure-state ensembles. Experimentally, such ensembles cannot be distinguished using the measurement statistics extracted via POVMs.

While this is all correct and familiar, we now demonstrate that it is, in fact, possible to distinguish these ensembles. The following gives a concrete scenario that clarifies how geometric quantum mechanics circumvents the information loss implicit in density matrix descriptions of quantum states. The result is a more accurate and complete theoretical description of a quantum experiment.

The scenario mimics a state-preparation protocol followed by state manipulation. There are two classical operators: Alice and Bob. Alice has a biased coin $\{H, T\}$, with $p_A(H) = (1+\lambda)/2$ and $p_A(T) = (1-\lambda)/2$, and two bags of qubit pure states. The first bag contains identical copies of $|0\rangle$, while the second contains identical copies of its orthogonal state $|1\rangle$. Each time she throws the coin, if Alice observes H she grabs a state from the first bag, otherwise she samples from the other. The result of this process is a state ensemble described by the density matrix:

$$\begin{aligned} \rho_A &= p_A(H) \, |0\rangle \langle 0| + p_A(T) \, |1\rangle \langle 1| \\ &= \frac{1}{2} \left(\mathbb{I} + \lambda \sigma_z \right) \ . \end{aligned} \tag{6}$$

To refine notation let $\left|\psi^A_H\right\rangle = |0\rangle$ and $\left|\psi^A_T\right\rangle = |1\rangle$.

Now, Bob is aware of Alice's classical bias λ and is interested in reproducing Alice's outcome. However, since he wants to experiment with quantum mechanics, he decides to stick to fair coins $p_B(H) = p_B(T) = \frac{1}{2}$, but uses quantum states with an overlap identical to the classical bias:

$$\left|\psi^B_H\right\rangle = \sqrt{\frac{1+\lambda}{2}} \, |0\rangle + \sqrt{\frac{1-\lambda}{2}} e^{i\chi} \, |1\rangle \ \text{ and} \tag{7a}$$

$$\left|\psi^B_T\right\rangle = \sqrt{\frac{1+\lambda}{2}} \, |0\rangle - \sqrt{\frac{1-\lambda}{2}} e^{i\chi} \, |1\rangle \ . \tag{7b}$$

Here, $\chi \in [0, 2\pi]$ is arbitrary and all states are legitimate quantum states that Bob can use.

Alice's bias $p_A(H) - p_A(T) = \lambda$ is the same as the *fidelity*:

$$|\left\langle \psi^B_H | \psi^B_T \right\rangle|^2 = \lambda \ .$$

Thus, Bob's experiment is described by the density matrix:

$$\rho_B = p_B(H) \left|\psi^B_H\right\rangle \left\langle \psi^B_H\right| + p_B(T) \left|\psi^B_T\right\rangle \left\langle \psi^B_T\right| \ .$$

By inspection one sees that Alice's an Bob's protocols give the same density matrix:

$$\begin{aligned}\rho_A &= \rho_B \\ &= \frac{1}{2}\left(\mathbb{I} + \lambda\sigma_z\right) \\ &= \begin{pmatrix} \frac{1+\lambda}{2} & 0 \\ 0 & \frac{1-\lambda}{2} \end{pmatrix} .\end{aligned}$$

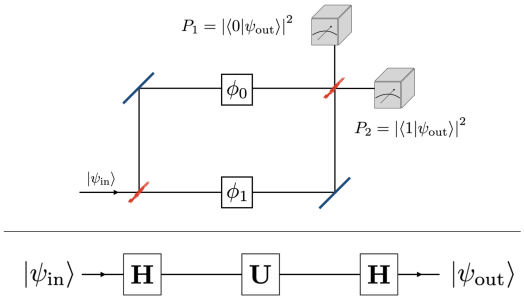

Figure 1. Interferometric detection scheme (upper) with its circuit representation (lower). An input state $|\psi_{\text{in}}\rangle$ passes through a beam splitter (left diagonal red line), reflects off two mirrors (blue diagonal lines), undergoes a phase-shift, with phase ϕ_0 in the upper path and ϕ_1 in the lower path, and eventually passes through a second beam splitter (right diagonal red line), and hits either detector 1 or 2. (We assume mirrors do not modify the system's state.)

Stepping back, shifting from Alice to Bob trades a classical source (Alice's) of randomness for one (Bob's) of quantum nature. However, invoking standard quantum mechanics, having the same density matrix one must conclude that there is no observable difference between the two protocols. In practice, this translates into the fact that the results of a quantum tomography protocol yield the same answer. Moreover, again by standard quantum mechanics, if we perform an information-processing task and then perform a measurement, we conclude that there is no discernible difference between the results of Alice's and Bob's protocols.

When the states resulting from both state-preparation protocols pass through an interferometer, as depicted in Fig. 1(upper), we model the output with the unitary operator $M = HUH$, where H is the Hadamard gate describing a beam-splitter:

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

and U is a phase-shift:

$$U = \begin{pmatrix} e^{i\phi_0} & 0 \\ 0 & e^{i\phi_1} \end{pmatrix} ,$$

from which only the difference $\phi_0 - \phi_1$ is observable. The interferometer is represented with the simple quantum circuit in Fig. 1(lower).

The statistics of the two detectors performing measurement in the computational basis is given by:

$$\begin{aligned} P_1^{(A)} &= \langle 0|\, M\rho_A M^\dagger\, |0\rangle \ , \\ P_2^{(A)} &= \langle 1|\, M\rho_A M^\dagger\, |1\rangle \ , \\ P_1^{(B)} &= \langle 0|\, M\rho_B M^\dagger\, |0\rangle \ , \text{ and} \\ P_2^{(B)} &= \langle 1|\, M\rho_B M^\dagger\, |1\rangle \ . \end{aligned}$$

Since $\rho_A = \rho_B$ we conclude that $P_i^{(A)} = P_i^{(B)}$, with:

$$P_1^{(A)} = \frac{1}{2} + \frac{\lambda}{2}\cos(\phi_0 - \phi_1) \text{ and} \tag{8a}$$

$$P_2^{(A)} = 1 - P_1^{(A)} \ . \tag{8b}$$

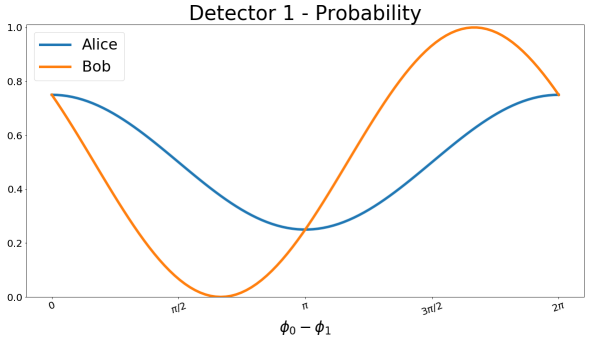

Figure 2. Probability of observing an event in detector 1 as a function of the phase-shift $\phi_0 - \phi_1$. Alice (blue) and Bob (orange) protocol results are given by Eq. (8) and Eq. (10), respectively. Here, $\lambda = 0.5$ and $\chi = \frac{\pi}{2}$.

However, if instead of the description $\rho = \frac{1}{2}\left(\mathbb{I} + \lambda\sigma_z\right)$, use that of the geometric quantum state or, for that matter, the ρ_B functional form, differences between Alice and Bob arise. Calling $q_A(Z)$ and $q_B(Z)$ the probability distribution on $\mathcal{P}(\mathcal{H})$ describing Alice's and Bob's states after they pass through the interferometer, respectively, one finds:

$$q_A(Z) = p_A(H)\widetilde{\delta}(Z - Z_H^A) + p_A(T)\widetilde{\delta}(Z - Z_T^A) \text{ and} \tag{9a}$$

$$q_B(Z) = p_B(H)\widetilde{\delta}(Z - Z_H^B) + p_B(T)\widetilde{\delta}(Z - Z_T^B) \ , \tag{9b}$$

where $Z^A_{H(T)}$ is such that:

$$\left|\psi^A_{H(T)}\right\rangle = \sum_{k=0}^{1}\left(Z^A_{H(T)}\right)_k |k\rangle \ .$$

Similar relations hold for $Z^B_{H(T)}$.

With these geometric quantum states we can compute the probability of a photon ending up in detectors using the geometric formalism described above. For detector 1, the results are:

$$\widetilde{P}_1^{(A)} = p_A(H)|\langle 0|M|\psi_H^A\rangle|^2 + p_A(T)|\langle 0|M|\psi_T^A\rangle|^2 \text{ and}$$
$$\widetilde{P}_1^{(B)} = p_B(H)|\langle 0|M|\psi_H^B\rangle|^2 + p_B(T)|\langle 0|M|\psi_T^B\rangle|^2 .$$

This gives the expected result $\widetilde{P}_1^{(A)} = P_1^{(A)}$ from Eq. (8). While for $\widetilde{P}_1^{(B)} \neq P_1^{(B)}$ one finds:

$$\widetilde{P}_1^{(B)} = \frac{1}{2} + \frac{\lambda}{2}\cos(\phi_0 - \phi_1) - \sqrt{\frac{1-\lambda^2}{4}}\sin(\phi_0 - \phi_1)\sin\chi. \tag{10}$$

Figure 2's plots of these probabilities as a function of phase shift $\phi_0 - \phi_1$ clearly reveals the differences between $\widetilde{P}_1^{(A)} = P_1^{(A)} = P_1^{(B)}$ and $\widetilde{P}_1^{(B)}$.

Concluding remarks. Conventional quantum mechanics harbors a degeneracy caused by the fact that two physically-distinct ensembles can have the same density matrix, as Alice and Bob did. Limiting ourselves to the statistics of POVM outcomes, this is not an issue. Indeed, one can check that the POVM statistics of Alice and Bob are the same. However, if we use the density matrix $\rho = \frac{1}{2}(\mathbb{I} + \lambda\sigma_z)$ to address the information-processing task described by Fig. 1's circuit, we are misled and arrive at incorrect predictions. This highlights a serious shortcoming of conventional quantum mechanics: Holding up the density matrix as the sole descriptor of a system's state brings down on ourselves the error of ignoring how an ensemble is realized in practice. Most directly, this has severe consequences when analyzing information-processing tasks that occur, for example, when a state ensemble passes through a quantum channel.

The geometric formalism provides an elegant, rigorous, and more inclusive alternative to the standard vector-based formalism of quantum mechanics. Its geometric quantum state is a probability distribution on the manifold of pure states and, in needed, density matrices can be computed as quadratic averages via Eq. (5). We emphasized a key advantage of the geometric formalism: It encodes both density matrix information, about all POVM statistics, and the ensemble realization. As a result, one can distinguish between different quantum states having the same POVM outcome statistics. This is particularly germane for quantum information and quantum computation since the distinct ensemble realizations of a density matrix are key to appropriately predicting the results of information processing tasks. Moreover, the alternative is also important for tasks of classical simulations of quantum phenomena as, inherently, our software largely calculates based on the matrix representation of a density operator that, again, does not encode the information about an ensemble's physical realization.

The lessons are simple. While the density matrix correctly captures all possible POVMs outcome statistics, it is not a complete description of the "state of the system". Rather, this role is appropriately played by the *geometric quantum state*.

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* fanza@ucdavis.edu
† chaos@ucdavis.edu

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