

Beyond Density Matrices: Geometric Quantum States

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In quantum mechanics, states are described by density matrices. 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, the outcome statistics of projective and positive operator-valued measurements do not depend on the ensemble realization, only on the density matrix. Here, we show how the geometric approach to quantum mechanics tracks ensemble realizations. We do so in two concrete cases of a finite-dimensional quantum system interacting with another one with (i) finite-dimensional Hilbert space, relevant for quantum thermodynamics, and (ii) infinite-dimensional Hilbert space, relevant for state-manipulation protocols.

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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 the probability distributions they support—Sinai-Bowen-Ruelle (SRB) measures on the system’s state space—are interpreted as the analogs of thermodynamic macrostates [1, 2]. Therein lie the foundations of classical statistical mechanics.

Building on this, the following introduces tools aimed at studying analogously-important state-space structures 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 SRB measures, they are specified by a probability distribution on the space of pure 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*. To account for more general situations, 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* [3, 4]. 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. 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 imagine systems that, despite being in obviously different physical situations, are described by the same density matrix. For example, consider two distinct state-preparation protocols. In one case, we prepare $\{|0\rangle, |1\rangle\}$ with classical probabilities $p_{0/1} = \frac{1 \pm \lambda}{2}$; in the other, we prepare states

$$|\psi_0\rangle = \sqrt{\frac{1+\lambda}{2}} |0\rangle + \sqrt{\frac{1-\lambda}{2}} e^{i\chi} |1\rangle, \quad (2a)$$

$$|\psi_1\rangle = \sqrt{\frac{1+\lambda}{2}} |0\rangle + \sqrt{\frac{1-\lambda}{2}} e^{i(\chi+\pi)} |1\rangle, \quad (2b)$$

each with probability 1/2. It is easy to check that they are described by the same ρ . It is also easy to see that the two state-preparation protocols simply traded a classical source of randomness, the bias $p_0 - p_1 = \lambda$, for one of quantum nature, the bias $|\langle \psi_0 | \psi_1 \rangle|^2 = \lambda$.

The following argues that an alternative—the *geomet-*

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ric formalism—together with an appropriately adapted measure theory overcomes these ambiguities.

With this perspective in mind, first, we recall the basics of *geometric quantum mechanics* (GQM) and discuss how it relates to density matrices. Then, we analyze two broad settings in which the geometric approach arises naturally. This is our main contribution. We consider a quantum system with a finite-dimensional Hilbert space that interacts with another one with (i) an infinite-dimensional Hilbert space and (ii) a finite-dimensional Hilbert space. These are relevant, respectively, for quantum state manipulation [5] and quantum thermodynamics [6]. With the results in hand, we draw out several consequences, including an alternative quantum foundation for thermodynamics that leads to quantitatively distinct predictions.

Geometric quantum mechanics. References [7–25] 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 $\mathcal{P}(\mathcal{H}) = \mathbb{CP}^{D-1}$. Therefore, given an arbitrary basis $\{|e_\alpha\rangle\}_{\alpha=0}^{D-1}$, a pure state 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 probability-phase coordinates $Z = (\sqrt{1-p}, \sqrt{p}e^{i\nu})$.

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

$$\mathcal{O}(Z) = \frac{\sum_{\alpha,\beta} \mathcal{O}_{\alpha,\beta} Z^\alpha \bar{Z}^\beta}{\sum_\gamma |Z^\gamma|^2} , \quad (3)$$

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 [26, 27]. 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:

$$E_j(Z) = \frac{\sum_{\alpha,\beta} (E_j)_{\alpha,\beta} Z^\alpha \bar{Z}^\beta}{\sum_\gamma |Z^\gamma|^2} , \quad (4)$$

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

The projective Hilbert space $\mathcal{P}(\mathcal{H})$ of a quantum system's pure states has a preferred metric g_{FS} —the *Fubini-Study metric* [17]—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 in the following:

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

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 natural to view a quantum state as a functional encoding that associates expectation values to observables, paralleling the C^* -algebra formulation of quantum mechanics [28]. The idea is that one considers probability density functions $q(Z)$ on $\mathcal{P}(\mathcal{H})$, together with observable functions $\mathcal{O}(Z)$. This was introduced in Ref. [16] 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, 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:

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

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.

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 these 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 Ref. [29]. References [6, 30] investigated its role in establishing a quantum foundation of thermodynamics distinct from 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. (4), 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 $Q = \int_{\mathbb{CP}^1} dV_{FS} e^{-\frac{1}{2} Z \rho^{-1} \bar{Z}}$, $Z_+ = (0.657, 0.418 + i0.627)$, 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.

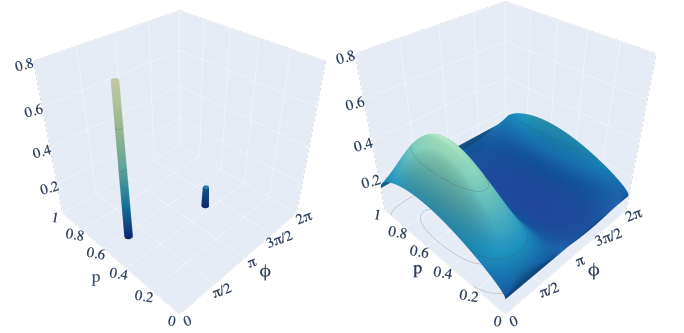


Figure 1. Geometric quantum states in $(probability, phase)$ coordinates (p, ϕ) of \mathbb{CP}^1 : (Left) Geometric quantum state q_1 is the convex sum of two Dirac delta-functions, centered on the eigenvectors $(p_+, \phi_+) = (0.568, 0.983)$ and $(p_-, \phi_-) = (0.432, 4.124)$ of density matrix ρ . (Right) Geometric quantum state q_2 differs markedly: A smooth distribution across the entire pure-state manifold \mathbb{CP}^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 $\rho_1 = \rho_2 = \rho$.

This is particularly important for quantum information processing where one encounters long-range and long-lived correlational and mechanistic constraints. 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 [31] 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 discrete. The entire system's Hilbert space is:

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

where $\mathcal{H}_N^c := \mathcal{H}_c^{\otimes N}$ hosts N one-dimensional continuous degrees of freedom and has infinite dimension, while $\mathcal{H}_M^d := \mathcal{H}_d^{\otimes M}$ hosts M discrete degrees of freedom, each with dimension d , and therefore 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 pure 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 $|\psi\rangle \in \mathcal{H}$ can be written as:*

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

where $f(\vec{x})$ is such that $\int_{\mathcal{R}} d\vec{x} |f(\vec{x})|^2 = 1$ and $\{|v(\vec{x})\rangle\}_{\vec{x}}$ is a set of states in \mathcal{H}_M^d , parametrized by \vec{x} and defined by:

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

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 (SM) gives the proof.)

Equation (8)'s pure-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:

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

Continuing, given an observable \mathcal{O} with support only on \mathcal{H}_M^d , we have:

$$\begin{aligned} \langle \mathcal{O} \rangle &= \text{Tr } \rho \mathcal{O} \\ &= \int_{\mathcal{R}} d\vec{x} |f(\vec{x})|^2 \mathcal{O}(v(\vec{x})) , \end{aligned} \quad (9)$$

where $\mathcal{O}(v(\vec{x})) = \langle v(\vec{x}) | \mathcal{O} | v(\vec{x}) \rangle$. Note that, here, the function $\mathcal{O}(\cdot)$ operates on $\mathcal{P}(\mathcal{H}_M^d)$ and it returns a real value. Thus, when we write $\mathcal{O}(v(\vec{x}))$ it means that, for each $\vec{x} \in \mathcal{R}$ there is an element, namely $v(\vec{x}) \in \mathcal{P}(\mathcal{H}_M^d)$, corresponding to the ket $|v(\vec{x})\rangle \in \mathcal{H}_M^d$, which is then the argument of $\mathcal{O}(\cdot)$ in $\mathcal{O}(v(\vec{x}))$. Thus, with an appropriate mathematical treatment we can turn the expectation value in Eq. (9) from an integral over \mathcal{R} into an integral over $\mathcal{P}(\mathcal{H}_M^d)$, with the appropriate measure being conveyed by an appropriately defined geometric quantum state.

To do so, we look at Eq. (5) and realize 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 $\mathcal{P}(\mathcal{H}_M^d)$ via:

$$\Phi : \vec{x} \in \mathcal{R} \longrightarrow \Phi(\vec{x}) = \Gamma(\vec{x}) \in \mathcal{P}(\mathcal{H}_M^d) ,$$

where $\Gamma = (\Gamma^0, \dots, \Gamma^\alpha, \dots, \Gamma^{d^M-1})$ with $\Gamma^\alpha(\vec{x}) = \sqrt{p_\alpha(\vec{x})} e^{i\phi_\alpha(\vec{x})}$. Thus, letting $\mathcal{R}^* = \Phi(\mathcal{R})$, we obtain:

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

In this:

$$q(Z) = \frac{|\det D\Phi(Z)|}{\sqrt{\det g_{FS}}} |f(\Phi^{-1}(Z))|^2 \quad (10)$$

takes into account the change in coordinates resulting from the embedding of \mathcal{R} on $\mathcal{P}(\mathcal{H}_M^d)$. Here, $D\Phi$ denotes the Jacobian of the transformation Φ , 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.

The SM provide a pedagogical example in the familiar case of a single electron in a 2D box.

In short, a generic ket $|\psi\rangle \in \mathcal{H}_N^c \otimes \mathcal{H}_M^d$ of the whole system uniquely defines a geometric quantum state $q(Z)$ on $\mathcal{P}(\mathcal{H}_M^d)$. The correspondence is not one-to-one as knowing $q(Z)$ does not allow recovering the entire state. The missing part is $\theta_0(\vec{x})$ —that is, $f(\vec{x})$'s phase. However, $q(Z)$ does circumscribe the possible realizations as it

fixes the shape of the continuous variables' probability distribution $|f(\vec{x})|^2$.

Imagine now that we wish to use the continuous degrees of freedom to manipulate or control the discrete ones and generate a specific geometric quantum state. There are clearly tradeoffs regarding how many qudits we can control with N one-dimensional, continuous-variable quantum systems. The functions $p_s(\vec{x})$ and $\phi_s(\vec{x})$ play the key role, as they determine the embedding. If we wish to control M qudits we need $2(d^M - 1)$ independent real coordinates. These must be supplied by the $2(d^M - 1)$ independent embedding functions $(p_s(\vec{x}), \phi_s(\vec{x}))$. Hence, if we have M qudits and N one-dimensional, continuous-variable, quantum systems, this means that there is a maximum number M_{\max} of qudits we can control, determined by $N = 2(d^{M_{\max}} - 1)$:

$$M \leq M_{\max} = \frac{\log(N/2 + 1)}{\log d}.$$

Thermodynamic framework. Another setting in which the geometric approach arises naturally is quantum thermodynamics; specifically when a finite-dimensional quantum system interacts with another with a finite-dimensional, but otherwise arbitrarily large, Hilbert space. For example, one is often interested in modeling the behavior of a small system interacting with a larger environment. For modest-sized environments one can treat the system and environment as isolated and then simulate their evolution. As the environment's size grows, though, 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. Theorem 1 guarantees this can be done.

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 ket 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, d_E is the dimension of the environment's Hilbert space, and d_S that of the system under study.

Given $|\psi_{SE}\rangle$, it is not too hard to see that the system's density matrix is:

$$\rho^S = \sum_{\alpha=1}^{d_E} p_\alpha^S |\chi_\alpha^S\rangle \langle \chi_\alpha^S|, \quad (11)$$

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 kets becomes quickly unrealistic.

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

$$p_{d_E}^S(Z) = \sum_{\alpha=1}^{d_E} p_\alpha^E \tilde{\delta}[Z - Z(\chi_\alpha^S)] \quad (12)$$

and the thermodynamic limit is handled with $p_\infty(Z) = \lim_{d_E \rightarrow \infty} p_{d_E}^S(Z)$.

Properly defining this limit requires addressing two issues. First, we must specify the iterative procedure to increase d_E in an operationally meaningful sense. Second, we must define the limit for the geometric quantum state. And, this requires a distance $D(\cdot, \cdot)$ between geometric quantum states that allows us to show that, given an arbitrarily small $\epsilon > 0$, there is always a $\bar{d}_E(\epsilon)$ such that for each $d_E > \bar{d}_E$ we have $D(p_{d_E}^S, p_\infty^S) \leq \epsilon$.

First, we define the operational sense behind the limit $d_E \rightarrow \infty$, for modular systems, with the following procedure. Modular indicates that the system consists of several subsystems of the same kind, described by copies of the same Hilbert spaces \mathcal{H}_d of dimension d . Thus, we imagine N_S subsystems comprising the system of interest and $N_E \geq N_S$ comprising the growing environment. Iteratively, starting with $N_E = N_S$ increase N_E by 1 unit and choose an element $|\psi_{SE}(N_E)\rangle$ of $\mathcal{H}_{SE}(N_E) = \mathcal{H}_d^{\otimes N_S} \otimes \mathcal{H}_d^{\otimes N_E}$. This procedure defines a series $\{|\psi_{SE}(N_E)\rangle\}_{N_E}$ and the only requirement for this series to provide a sensible operational definition for the thermodynamic limit is that the limit of the average energy density has to be finite: $\lim_{N_E \rightarrow \infty} \langle H_{SE} \rangle / (N_S + N_E) = \epsilon$, but it is otherwise arbitrary. Here, H_{SE} is the Hamiltonian of the whole system.

At each finite value of N_E , the treatment discussed above provides a well-defined set $\{(p_\alpha, |\chi_\alpha\rangle)\}_{\alpha=1}^{d^{N_E}}$ and, via Eq.(12), a well-defined geometric quantum state. Whether or not the procedure return, in the limit, a well-defined

geometric quantum state $p_\infty(Z)$ will depend on the system at hand and the particular choice of $\{|\psi_{SE}(N_E)\rangle\}_{N_E}$. For example, one can imagine to fix a specific form of the Hamiltonian (say, the XXZ model) and at each iteration pick the ground state of the Hamiltonian: $|G(N_E)\rangle$, such that $H_{SE}|G(N_E)\rangle = E_{\min}(N_E)|G(N_E)\rangle$. This provides a well-defined and physically meaningful operational procedure to study the thermodynamic limit.

In this way, the geometric formalism emerges naturally in a quantum thermodynamics setting. In the limit of large environments, one simply cannot track exactly how an environment generates the ensemble of our system under study and so, per force, switches to a probabilistic description. The geometric formalism handles this with the geometric quantum state $p_\infty(Z)$, or its approximations, that result from the thermodynamic limit procedure.

Second, we address the issue of an appropriate distance $D(\cdot, \cdot)$ to rigorously define the limit. Here, we choose D to be the total variation distance [32], defined as follows. Call \mathcal{B} the class of Borel sets on $\mathcal{P}(\mathcal{H})$. These are all sets that can be formed starting with open sets of $\mathcal{P}(\mathcal{H})$ via countable union, countable intersection, and relative complement. Given a geometric quantum state q and a set $A \in \mathcal{B}$, its measure is defined as follows:

$$\mu_q(A) := \int_A dV_{FS} q(Z) .$$

Given two geometric quantum states, q and p , with the respective measures μ_q and μ_p , the total variation distance between them is:

$$D(p, q) := \sup_{A \in \mathcal{B}} |\mu_q(A) - \mu_p(A)| .$$

This completes the definition of the thermodynamic limit. It properly frames the statement that, in certain cases, the iterative procedure defined above has a well-defined limit:

$$\lim_{d_E \rightarrow \infty} p_{d_E}^S(Z) = p_\infty^S(Z) .$$

Discussion and Conclusion. Quantum mechanics' concept of state is the density matrix. 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 [33], 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 a system under study, 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 more detailed system description—one that goes beyond the system's POVM statistics and takes into account the physical manner in which an ensemble has been realized.

After recalling the basics, above, we explored the benefits of the geometric approach in 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, but still finite-dimensional, environment.

We explicitly wrote the generic form of the system's geometric quantum state in these two cases. The geometric approach directly handles the continuous nature of hybrid systems and the large number of degrees of freedom in thermodynamics. And, it does so in a direct way, retaining the structural information about how an ensemble is generated. The result is a markedly richer picture of a quantum system's state—a picture that goes substantially beyond the density matrix and its POVM statistics.

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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* [34] and Schrodinger's *wave functions* [35] to von Neumann's *statistical operators* in Refs. [36] and [37, Chap. IV], later labeled *density matrices* by Dirac [38–40]. And, these were paralleled by Heisenberg's “operational” *matrix mechanics* that focused on experimentally accessible observables and so avoided imputing internal, hidden structure [41].

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

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

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

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

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

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 $\phi_s(\vec{x})$. To do so, first we define $\theta_s(\vec{x})$ as the phase of $\psi_s(\vec{x})$:

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

Starting from Eq. (B1) this gives:

$$|\psi\rangle = \int_{\mathcal{R}} d\vec{x} \sum_s \psi_s(\vec{x}) |\vec{x}\rangle |s\rangle = \int_{\mathcal{R}} d\vec{x} \sum_s |\psi_s(\vec{x})| e^{i\theta_s(\vec{x})} |\vec{x}\rangle |s\rangle . \quad (\text{B2})$$

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

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

With these definitions, assuming $\sum_{l=0}^{d^M-1} |\psi_l(\vec{x})|^2 \neq 0$, we can go through the following chain of equalities:

$$\begin{aligned} \psi_s(\vec{x}) &= \sqrt{|\psi_s(\vec{x})|^2} e^{i\theta_s(\vec{x})} \\ &= e^{i\theta_0(\vec{x})} |\psi_s(\vec{x})| e^{i(\theta_s(\vec{x}) - \theta_0(\vec{x}))} \\ &= e^{i\theta_0(\vec{x})} |\psi_s(\vec{x})| e^{i\phi_s(\vec{x})} \\ &= e^{i\theta_0(\vec{x})} |\psi_s(\vec{x})| e^{i\phi_s(\vec{x})} \frac{\sqrt{\sum_{l=0}^{d^M-1} |\psi_l(\vec{x})|^2}}{\sqrt{\sum_{l=0}^{d^M-1} |\psi_l(\vec{x})|^2}} \\ &= e^{i\phi_s(\vec{x})} \left(\sqrt{\sum_{l=0}^{d^M-1} |\psi_l(\vec{x})|^2} e^{i\theta_0(\vec{x})} \right) \left(\frac{|\psi_s(\vec{x})|}{\sqrt{\sum_{l=0}^{d^M-1} |\psi_l(\vec{x})|^2}} \right) \\ &= e^{i\phi_s(\vec{x})} f(\vec{x}) \sqrt{p_s(\vec{x})} . \end{aligned}$$

Hence:

$$\begin{aligned} |\psi\rangle &= \int_{\mathcal{R}} d\vec{x} \sum_s \psi_s(\vec{x}) |\vec{x}\rangle |s\rangle \\ &= \int_{\mathcal{R}} d\vec{x} \sum_s f(\vec{x}) \sqrt{p_s(\vec{x})} e^{i\phi_s(\vec{x})} |\vec{x}\rangle |s\rangle \\ &= \int_{\mathcal{R}} d\vec{x} f(\vec{x}) |\vec{x}\rangle \left(\sum_s \sqrt{p_s(\vec{x})} e^{i\phi_s(\vec{x})} |s\rangle \right) . \end{aligned} \quad (\text{B3})$$

At this point we note that $|f(\vec{x})|^2$ and $p_s(\vec{x})$ are normalized, in the following sense:

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

And so, for each $\vec{x} \in \mathcal{R}$, $|v(\vec{x})\rangle$, defined as follows, is an element of \mathcal{H}_M^d :

$$|v(\vec{x})\rangle := \sum_s \sqrt{p_s(\vec{x})} e^{i\phi_s(\vec{x})} |s\rangle \in \mathcal{H}_M^d .$$

In turn, this gives the desired result:

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

Appendix C: Electron in a 2D box

A familiar system will serve to illustrate: an electron in a 2D rectangular box $\mathcal{R}_{2D} = [x_0, x_1] \times [y_0, y_1]$. In this case $N = 2$, due to 2 spatial dimensions, and $M = 1$, $d = 2$. Thus, the discrete degrees of freedom of the system, just the spin-1/2 in this case, is described by $f(x, y)$ and $\{p_s(x, y), \phi_s(x, y)\}_{s=0,1}$. In this case, Eq.(9) becomes:

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

where, $p_0(x, y) = 1 - p_1(x, y)$, $p_1(x, y) = p(x, y)$, $\phi_0(x, y) = 0$, and $\phi_1(x, y) = \phi(x, y)$.

As concrete example let $p(x, y) = \frac{x-x_0}{x_1-x_0}$, $\phi(x, y) = 2\pi \frac{y-y_0}{y_1-y_0}$, and $f(x, y) = \sqrt{G(x, y)}$, where $G(x, y)$ is a 2D Gaussian on \mathcal{R}_{2D} :

$$G(x, y) = \begin{cases} \frac{e^{-\frac{1}{2}\left(\frac{x-\mu_x}{\sigma_x}\right)^2}}{\mathcal{N}_x} \frac{e^{-\frac{1}{2}\left(\frac{y-\mu_y}{\sigma_y}\right)^2}}{\mathcal{N}_y} , & (x, y) \in \mathcal{R}_{2D} \\ 0 , & \text{otherwise} \end{cases} ,$$

where (μ_x, σ_x) and (μ_y, σ_y) are the average and variance along the x and y axis, respectively. \mathcal{N}_x and \mathcal{N}_y are normalization factors.

Using the definitions of the embedding functions, we obtain the following set of spin vectors, parametrized by $\vec{x} = (x, y)$:

$$|v(x, y)\rangle = \sqrt{\frac{x_1 - x}{x_1 - x_0}} |0\rangle + \sqrt{\frac{x - x_0}{x_1 - x_0}} e^{i2\pi \frac{y-y_0}{y_1-y_0}} |1\rangle .$$

In turn, this gives:

$$\begin{aligned} \mathcal{O}(v(x, y)) &= \langle v(x, y) | \mathcal{O} | v(x, y) \rangle \\ &= \frac{x_1 - x}{x_1 - x_0} \mathcal{O}_{00} + \frac{x - x_0}{x_1 - x_0} \mathcal{O}_{11} + \sqrt{\frac{x_1 - x}{x_1 - x_0} \frac{x - x_0}{x_1 - x_0}} \left(\mathcal{O}_{01} e^{i2\pi \frac{y-y_0}{y_1-y_0}} + \frac{x - x_0}{x_1 - x_0} e^{-i2\pi \frac{y-y_0}{y_1-y_0}} \mathcal{O}_{10} \right) . \end{aligned}$$

The determinant of the Jacobian matrix between the coordinates (x, y) on \mathcal{R}_{2D} and $(p, \phi) \in [0, 1] \times [0, 2\pi]$ parametrizing $\mathcal{P}(\mathcal{H}_1^2) \sim \mathbb{CP}^1$ is extracted inverting the functions $p(x, y)$ and $\phi(x, y)$:

$$\begin{aligned} x(p, \phi) &= x_0 + p(x_1 - x_0) \\ y(p, \phi) &= y_0 + \frac{\phi}{2\pi} (y_1 - y_0) . \end{aligned}$$

This gives $D\Phi(Z) = (x_1 - x_0)(y_1 - y_0)/2\pi$, which in this case is a constant. Then, we have, as expected:

$$\begin{aligned}\mathcal{O}(v(x, y)) &= \mathcal{O}(v(x(p, \phi), y(p, \phi))) \\ &= (1 - p)\mathcal{O}_{00} + p\mathcal{O}_{11} + \sqrt{p(1 - p)} (\mathcal{O}_{01}e^{i\phi} + \mathcal{O}_{10}e^{-i\phi})\end{aligned}$$

and

$$G(x(p, \phi), y(p, \phi)) = \begin{cases} \frac{1}{\mathcal{N}_x} \exp \left[-\frac{1}{2} \left(\frac{x_0 + p(x_1 - x_0) - \mu_x}{\sigma_x} \right)^2 \right] \frac{1}{\mathcal{N}_y} \exp \left[-\frac{1}{2} \left(\frac{y_0 + \frac{\phi}{2\pi}(y_1 - y_0) - \mu_y}{\sigma_y} \right)^2 \right] , & (p, \phi) \in [0, 1] \times [0, 2\pi] \\ 0 , & \text{otherwise} \end{cases} .$$

Eventually, using Eq.(10) and $\sqrt{\det g_{FS}(p, \phi)} = 1/2$ and calling $G(x(p, \phi), y(p, \phi)) = \tilde{G}(p, \phi)$, the geometric quantum state is:

$$\begin{aligned}q(p, \phi) &= \frac{(x_1 - x_0)(y_1 - y_0)}{2\pi} \times 2 \times \tilde{G}(p, \phi) \\ &= \frac{(x_1 - x_0)(y_1 - y_0)}{\pi} \tilde{G}(p, \phi) .\end{aligned}$$

This can be written as:

$$q(p, \phi) = 2 \frac{1}{\mathcal{N}_p} \exp \left[-\frac{1}{2} \left(\frac{\mu_p - p}{\sigma_p} \right)^2 \right] \frac{1}{\mathcal{N}_\phi} \exp \left[-\frac{1}{2} \left(\frac{\phi - \mu_\phi}{\sigma_\phi} \right)^2 \right] , \quad (p, \phi) \in [0, 1] \times [0, 2\pi]$$

with $\mathcal{N}_p := \int_0^1 dp \exp \left(-\frac{1}{2} \left(\frac{p - \mu_p}{\sigma_p} \right)^2 \right)$, $\mathcal{N}_\phi := \int_0^{2\pi} d\phi \exp \left(-\frac{1}{2} \left(\frac{\phi - \mu_\phi}{\sigma_\phi} \right)^2 \right)$, and:

$$\begin{aligned}\mu_p &:= \frac{\mu_x - x_0}{x_0 - x_1} \\ \sigma_p &:= \frac{\sigma_x}{x_1 - x_0} \\ \mu_\phi &:= 2\pi \frac{\mu_y - y_0}{y_0 - y_1} \\ \sigma_\phi &:= \sigma_y \frac{2\pi}{y_1 - y_0} .\end{aligned}$$

$q(p, \phi)$ is positive and we can check that it is normalized. Remembering that in (p, ϕ) coordinates we have $dV_{FS}^{(p, \phi)} = dpd\phi/2$ gives:

$$\begin{aligned}\int_{\mathcal{P}(\mathcal{H}_1^2)} dV_{FS} q(p, \phi) &= 2 \frac{1}{2} \int_0^1 dp \frac{1}{\mathcal{N}_p} e^{-\frac{1}{2} \left(\frac{p - \mu_p}{\sigma_p} \right)^2} \int_0^{2\pi} d\phi \frac{e^{-\frac{1}{2} \left(\frac{\phi - \mu_\phi}{\sigma_\phi} \right)^2}}{\mathcal{N}_\phi} \\ &= \frac{\mathcal{N}_p \mathcal{N}_\phi}{\mathcal{N}_p \mathcal{N}_\phi} \\ &= 1 .\end{aligned}$$