A kinetic theory of quantum information transport

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INTRODUCTION.

The study of transport phenomena is crucial to harness the dynamical properties of natural systems. In this sense, transport theories are phenomenological descriptions of the nonequilibrium behavior of a system. Well-known examples are the theories of transport of charge, mass and heat. Most of them, were originally formulated to understand macroscopic phenomena like (in the case of mass transport) the tendency of a system to transfer mass in order to minimise the concentration difference. Over time, they were put on more rigorous ground using statistical mechanics and kinetic theory. Most notably, Boltzmann used this approach to describe the behavior of gases, and explain the rise of macroscopic irreversibility from the underlying time-symmetric classical mechanics. After Boltzmann's work, the core idea of treating motion and interaction in a statistical way has led to innumerable advances, both of fundamental and applied nature. With the rise of quantum theory, these techniques have also been adapted to include quantum fluctuations, leading to improved descriptions of transport phenomena at the nanoscale. While nowadays the use of kinetic and transport theories is ubiquitous, these techniques have not been leveraged to study quantum information in closed and open quantum systems. Thus, in this work, we attempt to lay a bridge between the field of quantum information and that of transport theories. More accurately, here we provide a self-consistent theory to track the dynamical evolution of a quantum state (and its probability distribution) in nonequilibrium quantum systems. We do so by building a kinetic theory of quantum state evolution, on the quantum state space, both in closed and open configurations.

At the technical level, this is done by leveraging recent work [**?** **?**] on Geometric Quantum Mechanics: a differential-geometric approach to quantum mechanics that gets rid of the phase redundancy of the Hilbert space. The geometric formalism maps the Hilbert space onto a space of pure states that has the structure of a classical phase-space, with canonically conjugated coordinates.

The paper is organized as follows. In Section I we give a brief summary of GQM, and of the tools introduced in [**?** **?**], both of which are needed. In Section II we give the first result: a microscopic derivation of the continuity equation for the information transport in quantum systems, with appropriate, microscopic definitions for phenomenological quantities such as fluxes and sink/sources terms. In Section III we give the second result: a general equation of motion for the probability distribution that an open quantum system is found in one of its quantum states. In Section IV we provide a few concrete examples, supported by numerical analysis. Eventually, in Section V we provide a quick summary and draw some conclusions.

I. GEOMETRIC QUANTUM MECHANICS

References [**?** **?** **?** **?** **?** **?** **?** **?** **?** **?** **?** **?** **?** **?** **?** **?** **?** **?** **?**] 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. For the details of the derivations, we send the reader to the literature cited above.

Given an arbitrary basis $\{|e_n\rangle\}_{n=0}^{D-1}$, a pure state is parametrized by D complex homogeneous coordinates $Z = \{Z^n\}$, up to normalization and an overall phase:

$$|\psi\rangle = \sum_{n=0}^{D-1} Z^n \, |e_n\rangle \ .$$

Here and throughout the paper we will always use upper indices to identify different coordinates of the same point and lower indices to identify different point. This description is redundant since we can renormalize Z by multiplying it for a real number and a phase (hence a complex number) and we would get the same physical situation. Therefore, $Z \in \mathbb{C}^D$, $Z \sim \lambda Z$, and $\lambda \in \mathbb{C}/\{0\}$. This equivalence relation means pure states of a quantum are points in the complex projective manifold $\mathcal{P}(\mathcal{H}) = \mathbb{C}\mathrm{P}^{D-1}$. If the system consists of a single qubit, for example, one can always use probability-phase coordinates $Z = (\sqrt{1-p}, \sqrt{p}e^{i\nu})$. We will often refer to this coordinates as they play a particular role.

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Observables and POVMs. 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:

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

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) $\{E_j\}_{j=1}^D$ applied to a state [**?** **?**]. They are nonnegative operators $E_j \geq 0$, called *effects*, that sum up to the identity: $\sum_{j=1}^D E_j = \mathbb{I}$. In GQM they consist of nonnegative real functions $E_j(Z) \geq 0$ on $\mathcal{P}(\mathcal{H})$ whose sum is always unity:

$$E_j(Z) = \frac{\sum_{m,n} (E_j)_{m,n} Z^m \overline{Z}^n}{\sum_k |Z^k|^2} \ , \tag{2}$$

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

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 $Z^n = \sqrt{p_n} e^{i\nu_n}$ that we use for explicit calculations:

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

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 $p_0 = 1 - \sum_{n=1}^{D-1} p_n$ 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 $\{(p_n, \phi_n)\}$ one has that $\{p_n, \phi_n\} = \frac{1}{\hbar}\delta_{nm}$. Thus, for arbitrary functions A and B on $\mathcal{P}(\mathcal{H})$ one has

$$\{A, B\} \coloneqq \frac{1}{\hbar} \sum_{n=1}^{D-1} \frac{\partial A}{\partial p_n}\frac{\partial B}{\partial \phi_n} - \frac{\partial B}{\partial p_n}\frac{\partial A}{\partial \phi_n} \tag{3}$$

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 $E(p_n, \phi_n) = \langle\psi(p_n, \phi_n)|\,H\,|\psi(p_n, \phi_n)\rangle$ the expectation value of H on a generic state $|\psi(p_n, \phi_n)\rangle = \sum_{n=0}^{D-1} \sqrt{p_n} e^{i\phi_n} |e_n\rangle$ parametrized by (p_n, ϕ_n), the unitary of a generic function A on $\mathcal{P}(\mathcal{H})$ is given by

$$\frac{\partial A}{\partial t} = \{A, E\} \tag{4}$$

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

$$\frac{dp_n}{dt} = \frac{1}{\hbar}\frac{\partial E}{\partial \phi_n} \tag{5a}$$

$$\frac{d\phi_n}{dt} = -\frac{1}{\hbar}\frac{\partial E}{\partial p_n} \tag{5b}$$

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:

$$P_q[\mathcal{O}] = \int_{\mathcal{P}(\mathcal{H})} q(Z)\mathcal{O}(Z) dV_{FS} \ , \tag{6}$$

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 $p_0(Z) = \widetilde{\delta}\,[Z - Z_0]$:

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

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

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

where $Z^n = X^n + iY^n$. In (p_n, ν_n) coordinates this becomes simply:

$$\widetilde{\delta}(Z - Z_0) = \prod_{n=1}^{D-1} 2\delta(p_n - p_n^0)\delta(\nu_n - \nu_n^0) \ ,$$

where the coordinate-invariant nature of the functionals $P_q[\mathcal{O}]$ is now apparent. Extending by linearity, mixed states

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

are convex combinations of these Dirac-delta functionals:

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

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

$$P_{\text{mix}}\left[\mathcal{O}\right] = \sum_j \lambda_j \left\langle\lambda_j\right| \mathcal{O} \left|\lambda_j\right\rangle \ . \tag{7}$$

Equipped with this tools, one identifies the distribution $q(Z)$ of Eq. (6) 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:

$$Q_\beta = \int dV_{FS} e^{-\beta h(Z)} \ ,$$
$$h(Z) = \left\langle\psi(Z)\right| H \left|\psi(Z)\right\rangle \ ,$$

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 fairly straightforward. Since density matrices are a synthetic way of collecting measurement outcomes about POVMs, which functions of the form $A(Z) \propto \sum_{n,m} A_{nm} Z^n \overline{Z}^m$, given a generic geometric quantum state $q(Z)$ the associated density matrix ρ^qcan be simply computed as follows:

$$\begin{aligned}\rho^q_{mn} &= P_q[Z^m \overline{Z}^n] \\ &= \int_{\mathcal{P}(\mathcal{H})} dV_{FS}\, q(Z)\, Z^m \overline{Z}^n \ .\end{aligned} \tag{8}$$

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.

The GQS of an Open Quantum System. As shown above, if a system is in a pure state its GQS is simply a Dirac delta concentrated on a single point. However, if the system is in contact with an environment, this is not true anymore, unless they are exactly in a product state. In general, contact with the environment causes the lost of information about which pure state the system inhabits. Hence, we need a probability distribution for the state of our system: a geometric quantum state. The explicit derivation of the generic geometric quantum state for an open quantum system can be found in Ref.[**?**]. Here we simply give the result, without discussing the derivation. Given a system and its environment, we call $\{|a_j\rangle\}_{j=0}^{d_S-1}$ a basis for the Hilbert space $\mathcal{H}_S$ of the system (dimension d_S) and $\{|b_n\rangle\}_{n=0}^{d_E}$ a basis for the Hilbert space $\mathcal{H}_E$ of the environment (dimension d_E). Assuming system and environment are in a pure state $|\psi_{SE}\rangle = \sum_{j,\alpha} \psi_{j\alpha} |a_j\rangle |b_\alpha\rangle$, the geometric quantum state of the system is

$$q(Z) = \sum_{\alpha=0}^{d_E-1} x_\alpha \widetilde{\delta}\left(Z - Z(\chi_\alpha)\right) \ , \tag{9}$$

where

$$x_\alpha \coloneqq \sum_j \left|\psi_{j\alpha}\right|^2 \ , \tag{10a}$$

$$\left|\chi_\alpha\right\rangle = \sum_j \frac{\psi_{j\alpha}}{\sqrt{x_\alpha}} \left|a_j\right\rangle \in \mathcal{H}_S \ . \tag{10b}$$

Here x_α is the probability that the environment is in state $|b_\alpha\rangle$ and $\{|\chi_\alpha\rangle\}$ is a set of d_E states of the system which constitutes the discrete support of the geometric quantum state. The geometric quantum state in Eq.(9) provides the correct reduced density matrix of the system $\rho^S(\psi_{SE}) = \sum_\alpha x_\alpha \left|\chi_\alpha\right\rangle \left\langle\chi_\alpha\right|$.

Probability mass in a region of the state space. Before we proceed with the main result, we introduce here a notation that will be useful later. This is imported from measure theory. Given a region $A \subseteq \mathcal{P}(\mathcal{H})$, we have

$$\mu_t(A) = \int_A q_t(Z) dV_{FS} \tag{11}$$

This is what we mean by "Information contained in a certain region of the state space". $\mu_t(A)$ quantifies the

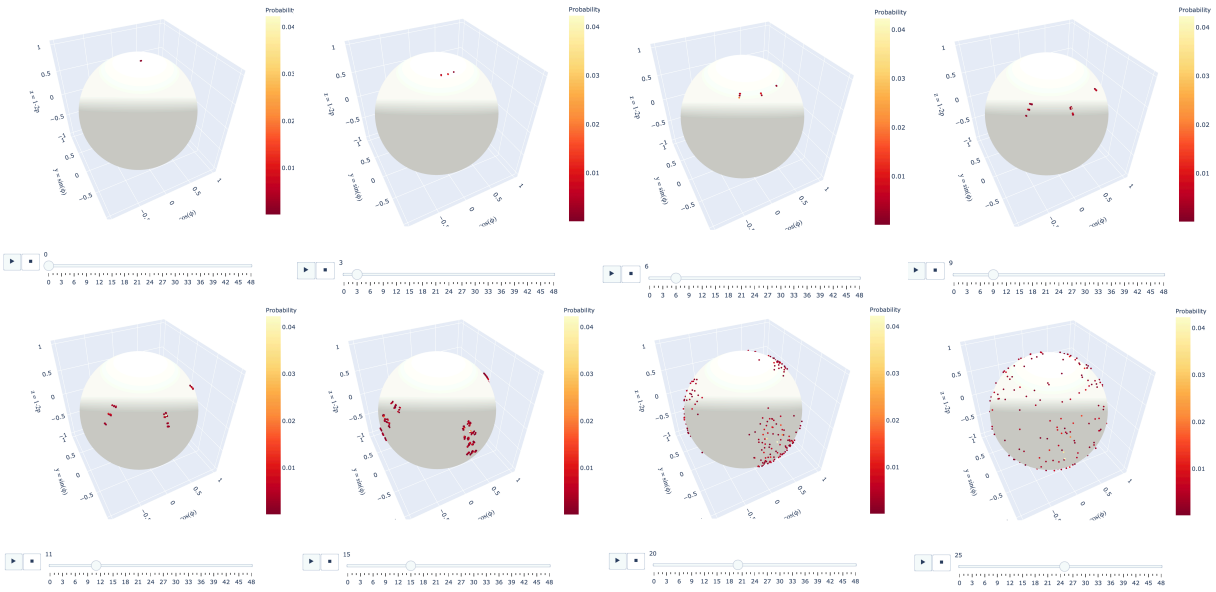

Figure 1. Evolution of the geometric quantum state of one qubit interacting with nine others via an Ising model with transverse field, visualized on the surface of the Bloch sphere. Each particle is $\Gamma_\alpha(t)$, represented in spherical coordinates $\Gamma_\alpha(t) = (\theta_\alpha(t), \phi_\alpha(t))$, with $|\psi(\theta,\phi)\rangle = \cos\theta/2\,|0\rangle + \sin\theta/2 e^{i\phi}\,|1\rangle$. The color of the point encodes the probability $x_\alpha(t)$. Time increases left to right and top to bottom. Each particle carries a probability mass x_α, which is the probability to find the system in a state Γ_α. Thus, we think of it as an information carrier, moving the information about the state of a quantum system around the quantum state space. The position of each particle is determined by the state of the environment and, indeed, there are 2^9 particles.

probability that, at time t, our quantum system is in a state Z that belongs to the region A of the quantum state space $\mathcal{P}(\mathcal{H})$.

II. INFORMATION TRANSPORT: CONTINUITY EQUATION

In the past section we have summarized previous results about GQM. In this section we build on them and, by bringing in the dynamics of the system, we derive a continuity equation which dictates how the geometric quantum state of a non-equilibrium open quantum system evolves, under very general assumptions. This is the fundamental kinetic equation that dictates how the information about the state of a quantum system changes as a result of its interaction with an environment. Throughout this section we will try to maintain a fairly general language, to emphasize how the treatment applies to quantum systems under very general assumptions. However, for concrete examples we will always refer to the simple case of a qubit.

General treatment

The following treatment pertains quantum systems which are finite-dimensional, and interact with finite-dimensional environments. Other than that, we continuity equation holds for arbitrary quantum systems.

Given an initial geometric quantum state, this is specified by two sets of quantities: $\{x_\alpha\}_{\alpha=0}^{d_E-1}$ and $\{\Gamma_\alpha\}_{\alpha=0}^{d_E-1}$, which is a short-hand notation for $\Gamma_\alpha = Z(|\chi_\alpha\rangle)$. The first one is a classical probability distribution resulting from hypothetical measurements on the environment. For each of the x_α there is a corresponding pure state that the system inhabits: $\Gamma_\alpha \in \mathcal{P}(\mathcal{H}_S)$, which corresponds to the ket $|\chi_\alpha\rangle$. Since these are points moving in a state space $\Gamma_\alpha(t)$, we can think of them as particles on a classical phases space, which interact in a non-trivial way. These are the "carriers of information", in the sense that each of these particles carries a probability mass $x_\alpha(t)$ that the system will be found on the state $\Gamma_\alpha(t)$. A clarifying example of how the geometric quantum state of a qubit evolves when the system interacts with an environment is given in Figure 1. Since the total amount of information has to be preserved, $\mu_t(\mathcal{P}(\mathcal{H})) = \int_{\mathcal{P}(\mathcal{H})} q_t(Z) dV_{\rm FS} = \sum_\alpha x_\alpha(t) = 1$, the geometric quantum state $q_t(Z)$ must satisfy a continuity equation. Conceptually, this is the starting point of virtually all transport theories, which deal with quantities that are globally conserved, but that are moved around as a result of the underlying dynamics.

Thus, the dynamics of a geometric quantum state has two different terms, arising from the time-evolution of these two sets of quantities. By looking at Figure 1 we can see that there are two different ways in which the

geometric quantum state changes in time. First, there is the color of each particle, which changes over time: $\dot{x}_\alpha \neq 0$. Second, there is the pure movements of each point: $\dot{\Gamma}_\alpha \neq 0$. By summing each term over all particles, and then summing the two terms, we get the following evolution equation for the geometric quantum state:

$$\frac{\partial q_t(Z)}{\partial t} = \sum_\alpha \dot{x}_\alpha \tilde{\delta}\left(Z - \Gamma_\alpha\right) - x_\alpha \widetilde{\delta}^{'}\left(Z - \Gamma_\alpha\right)\dot{\Gamma}_\alpha \ . \quad (12)$$

Here $\delta^{'}$ is the first distributional derivative of the dirac delta distribution. The second term in the right-hand side can be written as a covariant divergence[1], since every dipendence on the coordinate Z is inside the delta distribution:

$$\sum_\alpha x_\alpha \widetilde{\delta}^{'}\left(Z - \Gamma_\alpha\right)\dot{\Gamma}_\alpha = (\nabla \cdot J_t)(Z) \quad (13)$$

This allows us to identify the first functional term of the continuity equation, the *flux of information* $J(t)$, which is a weighted average of the "single-particle" flux $J_\alpha(t)$:

$$J_\alpha(t) = \widetilde{\delta}\left(Z - \Gamma_\alpha(t)\right)\dot{\Gamma}_\alpha(t) \ , \quad (14a)$$

$$J(t) = \sum_\alpha x_\alpha(t) J_\alpha(t) \ . \quad (14b)$$

We now look at the first term in the right-hand: $\sum_\alpha \dot{x}_\alpha(t)\delta(Z - \Gamma_\alpha(t))$. This is identified to be a source/sink term, which is independent on the underlying movement of the points in the quantum state space. This identifies the second functional term of our continuity equation: *sinks and sources of information* $\sigma_t(Z)$:

$$\sigma_t(Z) = \sum_{\alpha=0}^{d_E} \dot{x}_\alpha(t)\widetilde{\delta}\left(Z - \Gamma_\alpha(t)\right) \ . \quad (15)$$

Eventually, we obtain the following continuity equation for the geometric quantum state of a finite-dimensional quantum system interacting with a finite-dimensional environment:

$$\frac{\partial q_t}{\partial t} + \nabla \cdot J_t = \sigma_t \quad (16)$$

This is our first result. A crucial aspect here is that this theoretical framework allows us to talk about information as a physically localized (and overall conserved) quantity, which is carried around by points in quantum state space. This is in analogy with the classical theories of information, which deal with properties of particles such as mass or charge, which are carried around by particles, represented as points wondering in a classical phase-space.

To reinforce this point, the physical interpretation of the flux J_t and source/sink σ_t term is essentially the same as in other transport theories. We now describe them explicitly, together with their kinetic interpretation, drawn in Figures 2 and 3. First, J_t is an information flux, in the proper sense of flux. As one can appreciate in Figure 2, this flux is associated to an overall conserved quantity, localized in its carriers Γ_α, which move around and distribute it across the quantum state space. To emphasize this point we look at the simpler situation in which $\dot{x}_\alpha = 0$. In this case, the information carried around by the points in state space is a constant of motion ($x_\alpha(t) = x_\alpha(t_0)$). However, as the carriers move around, the information is still dispersed across the quantum state space. Second, the term σ_t is a proper source/sink term, with the usual interpretation. Indeed, we note that it can not be written as a divergence term. To emphasize this point we look at the simpler dynamics in which the position of the points in $\mathcal{P}(\mathcal{H})$ does not change: $\dot{\Gamma}_\alpha = 0$. In this case the support of the distribution is fixed and the particles don't move $\Gamma_\alpha(t) = \Gamma_\alpha(t_0)$. However, even in this case there can still be a non-trivial dynamics, due to $\dot{x}_\alpha(t) \neq 0$. Moreover, as depicted in Figure 3, the time-evolution generated by this term is generally non-local in the quantum state space. Thus, σ_t possesses all the hallmarks of the standard sinks and sources terms in general transport theories: it is not associated with particles moving around the state space and it can not be rewritten as a divergence term.

Closed quantum systems

What happens when the system is closed? Is there a specific form for the information flux J_t and source σ_t? Here we answer both these questions in a detailed manner. Since the evolution is Hamiltonian, we can use Hamilton's equations of motion to derive the evolution equation of μ_t or, equivalently, of $q_t(Z)$. First, the sink/sources terms is trivially zero, as the evolution is Hamiltonian and preserves the local probabilities. Second, starting from the definition of the flux in Eq.(14), we can explicitly write the form of the flux J_t, using Hamilton's equations of motion. Writing Γ_α in canonical coordinates $(p_n(\Gamma_\alpha), \phi_n(\Gamma_\alpha))$, we have

$$\begin{aligned}\dot{\Gamma}_\alpha &= \left\{\left(\dot{p}_n(\Gamma_\alpha), \dot{\phi}_n(\Gamma_\alpha)\right)\right\}_n \\ &= \left\{\frac{1}{\hbar}\left(\frac{\partial E}{\partial \phi_n}, -\frac{\partial E}{\partial p_n}\right)\right\}_n = v_H(p_n, \phi_n)\end{aligned} \quad (17)$$

Note how the right-hand side, which we called v_H does not depend on the index α anymore: all the points evolve in the same way, following the same Hamiltonian flow. Inserting this into the definition of the flux we obtain that the flux is equal to the product between the distribution

[1] With an arbitrary coordinate system we have $\mathrm{div}\vec{f} = \frac{1}{\sqrt{g}}\partial_\alpha\left(\sqrt{g} f^\alpha\right)$, where $g = |\det g_{FS}|$ is the absolute value of the determinant of the metric which, in our case, is the Fubini-Study metric.

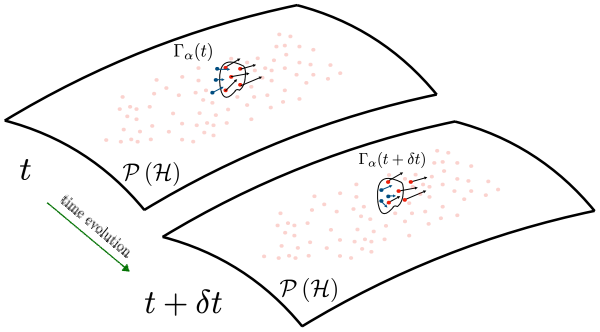

Figure 2. Kinetic interpretation of the flux J. If we look at a small region of the quantum state space, due to the underlying dynamics we see that information is locally conserved in the sense that there is a certain number of points which enters and leaves this region. As a result of this local process, probability is moved around and can concentrate in a certain region or get scrambled across the quantum state space.

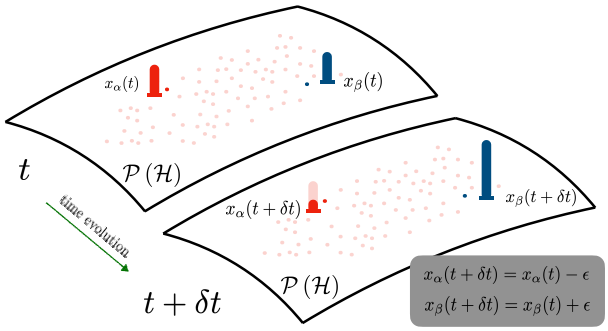

Figure 3. Kinetic interpretation of the sink/source term σ_t. Even if the points do not move around the quantum state space $\dot{\Gamma}_\alpha = 0$, the term σ_t allows the exchange of information between different regions. Note that this can be a non-local effect, as depicted above. In the example above we have two state Γ_α and Γ_β fixed in time, but exchanging a certain amount ϵ of probability, thus moving information from one region of the state space to another one: $x_\beta(t+\delta t) = x_\beta(t) + \epsilon$, $x_\alpha(t+\delta t) = x_\alpha(t) - \epsilon$.

and the Hamiltonian velocity field v_H:

$$J_t(Z) = q_t(Z) v_H(Z) \ , \tag{18}$$

thus providing the following continuity equation:

$$\frac{\partial q_t}{\partial t} = -v_H \cdot \nabla q_t - q_t \, \nabla \cdot v_H \tag{19}$$

This can be further simplified by noting that the Hamiltonian vector field is divergence free, $\nabla \cdot v_H = 0$. This is due to the smoothness of $E(p_n, \phi_n)$ which, via Schwarz's theorem, implies that the Hessian of $E(p_n, \phi_n)$ is symmetric.

$$\begin{aligned} \nabla \cdot v_H &= \sum_n \left(\frac{\partial}{\partial p_n}, \frac{\partial}{\partial \phi_n} \right) \cdot \frac{1}{\hbar} \left(\frac{\partial E}{\partial \phi_n}, -\frac{\partial E}{\partial p_n} \right) \\ &= \frac{1}{\hbar} \sum_n \left(\frac{\partial^2 E}{\partial p_n \partial \phi_n} - \frac{\partial^2 E}{\partial \phi_n \partial p_n} \right) = 0 \end{aligned}$$

This leads us to the final form of the continuity equation of an isolated quantum system:

$$\frac{\partial q_t}{\partial t} = -v_H \cdot \nabla q_t = -\{q_t, E\} \tag{20}$$

Liouville's theorem for GQM. As a further point of contact with the techniques of classical statistical mechanics and kinetic theory, we now show that a generic Hamiltonian dynamics for the geometric quantum state satisfies Liouville's theorem [**?**]. Indeed, by writing explicitly the total derivative of $q_t(Z)$ with respect to time we get

$$\frac{dq}{dt} = \sum_\alpha \frac{\partial q_t}{\partial p_\alpha} \frac{dp_\alpha}{dt} + \frac{\partial q_t}{\partial \phi_\alpha} \frac{d\phi_\alpha}{dt} + \frac{\partial q_t}{\partial t} \tag{21}$$

Inserting Hamilton's equations of motion (Eq. (5)), and then using the continuity equation

$$\begin{aligned} \frac{dq}{dt} &= \sum_\alpha \frac{\partial q_t}{\partial p_\alpha} \frac{dp_\alpha}{dt} + \frac{\partial q_t}{\partial \phi_\alpha} \frac{d\phi_\alpha}{dt} + \frac{\partial q_t}{\partial t} \\ &= \{q_t, E\} - \nabla \cdot q_t v_H = 0 \end{aligned} \tag{22}$$

This concludes the section about the general approach, and the treatment of isolated quantum systems. We now turn to the more pertinent, and involved, case of an open quantum system.

Discussion

- This kind of hamiltonian dynamics is more restrictive than a generic classical Hamiltonian dynamics: No chaos allowed, as the distance between points is constant.
- Hence, we can concot Hamiltonian dynamics that violate this condition, possibly to give us quantum chaos.
- Equilibrium ($J = \sigma = 0$) and non-equilibrium stationary states.

III. KINETIC THEORY OF INFORMATION TRANSPORT IN OPEN QUANTUM SYSTEMS

As we move to analyze how open quantum systems move information around the quantum state space, the goal of this section is to provide a microscopic approach to the transport of information: a kinetic theory of how

the information about the state of a quantum system changes as a result of its interaction with a structured, non-thermal, environment. Thus, the main outcome of this section is a concrete set of microscopic equations that determines the evolution of the geometric quantum state in a non-Hamiltonian setting.

Calling H_S and H_E the Hamiltonian operators of the system and environment, respectively, the total Hamiltonian of the joint system is $H = H_S + H_E + H_{\rm int}$. Since $H_{\rm int}$ is the interaction term between system and environment, we can always put it in the form

$$H_{\rm int} = \sum_{k=1}^{M} A^{(k)} \otimes B^{(k)} \ , \tag{23}$$

where $A^{(k)}$ and $B^{(k)}$ are operators with support on $\mathcal{H}_S$ and $\mathcal{H}_E$, respectively. With a slight abuse of notation we will often conflate $A^{(k)}$ with $A^{(k)} \otimes \mathbb{I}_E$ and $B^{(k)}$ with $\mathbb{I}_S \otimes B^{(k)}$, where $\mathbb{I}_S$ and $\mathbb{I}_E$ are, respectively, the identity operator on $\mathcal{H}_S$ and $\mathcal{H}_E$. Here we do not make a specific choice for the basis of the system and environment. While an obvious one is to choose the bases that diagonalize the non-interacting Hamiltonians H_S and H_E, there are cases where this is not required. For example, in the case of a spin-1/2 chain one might be interested in using the computational basis. Thus, we keep things general and use a generic basis, with no particular properties with respect to the algebra of observables: $\{|a_j\rangle\}_{j=0}^{d_S}$ and $\{|b_\alpha\rangle\}_{\alpha=0}^{d_E-1}$.

Since the goal is to derive a dynamic equation for $\{x_\alpha(t)\}$ and $\{\Gamma_\alpha(t)\}$, we begin with the overall Schroedinger equation for the pure state $|\psi(t)\rangle$ of the joint system+environment, written in the generic tensor product basis defined above, with $\psi_{j\alpha}(t) = \langle a_j, e_\alpha|\psi(t)\rangle$:

$$i\hbar \frac{d\psi_{j\alpha}(t)}{dt} = \sum_{k,\beta} H_{j\alpha;k\beta}\psi_{k\beta}(t) \ , \tag{24}$$

where

$$\begin{aligned} H_{j\alpha;k\beta} &= \langle a_j, b_\alpha| H |a_k, b_\beta\rangle \\ &= (H_S)_{jk}\,\delta_{\alpha\beta} + \delta_{jk}\,(H_E)_{\alpha\beta} + \sum_{n=1}^{M} A^{(n)}_{jk} B^{(n)}_{\alpha\beta} \ . \end{aligned} \tag{25}$$

We now collect the probability $x_\alpha(t)$ and the states $|\chi_\alpha(t)\rangle$ into a single quantity: a non-normalized ket $|\Phi_\alpha(t)\rangle \coloneqq \sqrt{x_\alpha}\,|\chi_\alpha\rangle \in \mathcal{H}_S$. By plugging Schroedinger's equation into the time-derivative of $|\Phi_\alpha(t)\rangle$ we get the following set of d_E interacting linear equations:

$$i\hbar \frac{d\,|\Phi_\alpha\rangle}{dt} = H_S\,|\Phi_\alpha\rangle + \sum_\beta (H_E)_{\alpha\beta}\,|\Phi_\beta\rangle + \hat{M}_{\alpha\beta}\,|\Phi_\beta\rangle \ , \tag{26}$$

where $\hat{M}_{\alpha\beta}$ is a set of operators acting on the system, defined as

$$\hat{M}_{\alpha\beta} = \sum_{k=1}^{M} B^{(k)}_{\alpha\beta} A^{(k)} \tag{27}$$

This can be further manipulated to separate the non-interacting part, acting on each vector $|\Phi_\alpha\rangle$, from the interacting part, acting on $|\Phi_\beta\rangle \neq |\Phi_\alpha\rangle$. The final form of our kinetic equation is

$$i\hbar \frac{d\,|\Phi_\alpha\rangle}{dt} = \hat{H}_\alpha\,|\Phi_\alpha\rangle + \sum_{\beta\neq\alpha} \hat{V}_{\alpha\beta}\,|\Phi_\beta\rangle \ , \tag{28}$$

where the single-particle Hamiltonian is $\hat{H}_\alpha$ is

$$\hat{H}_\alpha \coloneqq H_S + (H_E)_{\alpha\alpha}\,\mathbb{I}_S + \sum_{k=1}^{M} B^{(k)}_{\alpha\alpha} A^{(k)} \ , \tag{29}$$

and the interaction between particles is vehiculated by the set of operators $\hat{V}_{\alpha\beta}$

$$\hat{V}_{\alpha\beta} \coloneqq (H_E)_{\alpha\beta}\,\mathbb{I}_S + \sum_{k=1}^{M} B^{(k)}_{\alpha\beta} A^{(k)} \ . \tag{30}$$

The remaining step is to connect this with the quantities that determine the geometric quantum state of the system: x_α and Γ_α. This is easily done by using the original definition $|\Phi_\alpha\rangle = \sqrt{x_\alpha}\,|\chi_\alpha\rangle$. Since $\Gamma_\alpha(t) \leftrightarrow |\chi_\alpha\rangle$, we have $\Gamma^j_\alpha(t) = \frac{\langle a_j|\Phi_\alpha(t)\rangle}{\sqrt{x_\alpha(t)}}$ and $x_\alpha(t) = \langle\Phi_\alpha(t)|\Phi_\alpha(t)\rangle$.

This concludes the derivation of the microscopic kinetics of the points in quantum state space, for an open quantum system interacting with a finite-dimensional environment. While not treated here, by using the approach developed in Ref.[**?**] these results can be extended to include finite-systems interacting with infinite-dimensional environments.

First, as a consistency check, we note that the preservation of information within the quantum state space of the system is inherited by the unitarity of the global evolution. This is manifested in the relations $\hat{H}^\dagger_\alpha = \hat{H}_\alpha$ and $\hat{V}^\dagger_{\alpha\beta} = \hat{V}_{\beta\alpha}$, both of which can be easily shown to be true from the definitions above.

IV. CASE STUDIES

So far we have developed the microscopic, kinetic, equations regulating the information transport across the quantum state space. In this section we use an analytical and numerical approach to look at the information transport in concrete physical systems. In particular, in our examples we look at the information transport in the state space of a qubit. Both in isolated and open configuration. This choice is made to support the theoretical

calculations with visual representations, both of which are simpler in the case of a qubit.

State space of a qubit: Canonical coordinates

Before we begin our case studies, here we collect useful technical details about the geometric quantum mechanics of a qubit. First, we will be using units in which $\hbar = 1$. Then, using as a reference basis an arbitrary basis $\{|0\rangle, |1\rangle\}$ the (probability,phase) coordinates are identified via the following scalar product on the Hilbert space $\langle s|\psi\rangle = \sqrt{p_s}e^{i\phi_s}$, with $s = 0, 1$, giving $(p_0, \phi_0, p_1, \phi_1)$. However, the quantum state space gets rid of two fundamental redundancies in this description. First, we can always assume that $\phi_0 = 0$. Second, due to normalization we have $p_0 = 1 - p_1$. Thus, we only have a pair of independent coordinates: (p_1, ϕ_1). We can therefore drop the index and say that a general point on the state space of a qubit is uniquely identified by $(p, \phi) \in [0, 1] \times [0, 2\pi[$, with an embedding on the Hilbert space defined by $|\psi(p, \phi)\rangle = \sqrt{1-p}\,|0\rangle + \sqrt{p}e^{i\phi}\,|1\rangle$. Note that the embedding is smooth everywhere, aside for two isolated points $|0\rangle$ and $|1\rangle$, where ϕ is not defined and which are represented only by $p = 0$ and $p = 1$, respectively. These coordinates (p, ϕ) are canonically conjugated: $\{p, \phi\}$ and the determinant of the Fubini-Study metric is simply $g = \frac{1}{2}$. Moreover, since the total volume of the state space is π [], we renormalize the Fubini-Study volume element with the total volume, so that $dV = \frac{dpd\phi}{2\pi} = \frac{dV_{FS}}{\mathrm{Vol}(\mathbb{C}P^1)}$.

Isolated qubit

Our first case study is an isolated qubit, with an arbitrary initial geometric quantum state $f_0(p, \phi)$ and Hamiltonian operator $H = \vec{h} \cdot \vec{\sigma} = E_0 \,|E_0\rangle \langle E_0| + E_1 \,|E_1\rangle \langle E_1|$. Thus, the generator of the geometric evolution is:

$$\begin{aligned}\mathcal{E}(p, \phi) &= \langle \psi(p, \phi)| \, H \, |\psi(p, \phi)\rangle = (1-p)H_{00} + pH_{11} \\ &+ \sqrt{p(1-p)}\left(e^{i\phi}H_{01} + e^{-i\phi}H_{10}\right) \\ &= \vec{h} \cdot \vec{S} \ ,\end{aligned} \tag{31}$$

where

$$\vec{S} = \langle \vec{\sigma} \rangle = \left(2\sqrt{p(1-p)}\cos\phi, 2\sqrt{p(1-p)}\sin\phi, p\right) \tag{32}$$

Since the evolution is Hamiltonian, there is no source or sink term, so the continuity equation is

$$\frac{\partial f_t(p, \phi)}{\partial t} + \nabla \cdot J_t = 0 \ . \tag{33}$$

In canonical coordinates the ∇ operator is simply $\nabla = (\frac{\partial}{\partial p}, \frac{\partial}{\partial \phi})$. Writing explicitly, we get

$$\frac{\partial f_t(p, \phi)}{\partial t} + \frac{\partial J_t^p}{\partial p} + \frac{\partial J_t^\phi}{\partial \phi} = 0 \ . \tag{34}$$

We now come to writing explicitly the flux $J_t = (J_t^p, J_t^\phi)$. As argued above, with Hamiltonian evolution the flux is the product between the Hamiltonian vector field v_H and the geometric quantum state $f_t(p, \phi)$. Explicitly:

$$J_t = \frac{f_t(p, \phi)}{\hbar}\left(\frac{\partial \mathcal{E}(p, \phi)}{\partial \phi}, -\frac{\partial \mathcal{E}(p, \phi)}{\partial p}\right) \tag{35}$$

Plugging this into the continuity equation we get an equation for $f_t(p, \phi)$ and remembering that a Hamiltonian vector field is divergence-free, we get

$$\frac{\partial f_t}{\partial t} + A(p, \phi)\frac{\partial f}{\partial p} + B(p, \phi)\frac{\partial f}{\partial \phi} = 0 \ , \tag{36}$$

with $A(p, \phi) = \frac{1}{\hbar}\frac{\partial \mathcal{E}}{\partial \phi}$ and $B(p, \phi) = -\frac{1}{\hbar}\frac{\partial \mathcal{E}}{\partial p}$. This is a linear, first-order, partial differential equation, which can be solved in full generality by using the method of the characteristics. Here we simplify the treatment by switching to coordinates aligned to the convenient basis in which the Hamiltonian is diagonal. This leads to

$$\frac{\partial f}{\partial t} - \omega\frac{\partial f}{\partial \phi} = 0 \ , \tag{37}$$

where $\omega = \frac{E_1 - E_0}{\hbar}$. This is equivalent to the transport equation for advection, which leads the analytical solution for the time-dependent geometric quantum state: $f_t(p, \phi) = f_0(p, \phi + \omega t)$, for any valid initial distribution $f_0(p, \phi)$.

HERE

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. (8).

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 transport

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:

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

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

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

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:

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

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

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

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:

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