A kinetic theory of quantum information

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TBD

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. We do so by building a kinetic theory of quantum information for closed and open quantum systems. The main goal of this work is to provide a consistent definition for common tools such as fluxes and sink/sources which

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 ?? 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 ?? 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 ?? we provide a few concrete examples, supported by numerical analysis. Eventually, in Section ?? 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.

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 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:

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

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)

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$\{E_j\}_{j=1}^n$ applied to a state [? ?]. 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:

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

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

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

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

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

Geometric quantum states. This framework makes it very natural to view a quantum state as a functional encoding that associates expectation values to observables, paralleling the C^*-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:

$$P_q[\mathcal{O}] = \int_{\mathcal{P}(\mathcal{H})} q(Z)\mathcal{O}(Z)dV_{FS} \ , \qquad (3)$$

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

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

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

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

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

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

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:

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

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

$$P_{\text{mix}}[\mathcal{O}] = \sum_j \lambda_j \langle\lambda_j| \mathcal{O} |\lambda_j\rangle \ . \qquad (4)$$

Equipped with this tools, one identifies the distribution $q(Z)$ of Eq. (3) as a system's *geometric quantum state*. This is a generalized notion of quantum state.

A simple example of a geometric quantum state is the *geometric canonical ensemble*:

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

where:

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

and H is the system's Hamiltonian operator. This was introduced in Refs. [?]. References [?] and [?] investigated its potential role in establishing a quantum foundation of thermodynamics that is an alternative to that based on Gibbs ensembles and von Neumann entropy.

Density matrix. The connection between geometric quantum states and density matrices is two-fold. On the one hand, when $q(Z)$ falls into one of the two aforementioned cases—Dirac-deltas or finite convex combinations of them—the present formalism is equivalent to the standard one. However, not all functionals fall into the Dirac-delta form. Given this, $q(Z)$ is clearly a more general no-

tion 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:

$$\rho^q_{\alpha\beta} = P_q[Z^\alpha \overline{Z}^\beta]$$
$$= \int_{\mathcal{P}(\mathcal{H})} dV_{FS}\, q(Z)\, Z^\alpha \overline{Z}^\beta \;. \qquad (5)$$

Owing to the specific form of POVMs on $\mathcal{P}(\mathcal{H})$, recall Eq. (2), they are sensitive to $q(Z)$ only via ρ^q. Therefore, if two geometric quantum states q_1 and q_2 induce the same density matrix $\rho^{q_1} = \rho^{q_2}$, then all POVMs produce the same outcomes.

A well-known consequence of this fact is that two density matrices with the same barycenter are considered equal, even if they describe experiments with different physical configurations. In these cases, the statistics of POVM outcomes are described by the same density matrix. Note that this statement does not mean that the two physical configurations are the same. Rather, it means that there is no POVM on the system that distinguishes between q_1 and q_2.

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

$$q_1(Z) = 0.864\, \tilde{\delta}(Z - Z_+) + 0.136\, \tilde{\delta}(Z - Z_-)\;,$$
$$q_2(Z) = \frac{1}{Q} e^{-\frac{1}{2}\overline{Z}\rho^{-1}Z}\;,$$

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

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

SUMMARY.

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
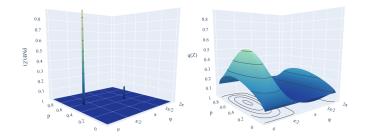

Figure 1. Geometric quantum states in *(probability,phase)* coordinates (p, ϕ) of $\mathbb{C}P^1$: (Left) Geometric quantum state q_1 is the convex sum of two Dirac delta-functions, centered on the eigenvectors $(p_+, \phi_+) = (0.568, 0.983)$ and $(p_-, \phi_-) = (0.432, 4.124)$ of density matrix ρ. (Right) Geometric quantum state q_2 differs markedly: A smooth distribution across the entire pure-state manifold $\mathbb{C}P^1$. However, q_1 and q_2 have the same density matrix $\rho_{q_1} = \rho_{q_2} = \rho$, where $\rho_{00} = 1-\rho_{11} = 0.45$, $\rho_{01} = \rho_{10}^* = 0.2-0.3i$. $\rho_\pm$ 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 $\rho_1 = \rho_2 = \rho$.

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. (5).

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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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

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

Starting from Eq.(B1) this gives

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

$$= \int_{\mathcal{R}} d\vec{x} e^{i\theta_0(\vec{x})} \sum_s |\psi_s(\vec{x})| e^{i\phi_s(\vec{x})} |\vec{x}\rangle |s\rangle$$

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

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

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

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

$$\int_{\mathcal{R}} d\vec{x} |f(\vec{x})|^2 = \int_{\mathcal{R}} d\vec{x} \sum_{s=0}^{d^M-1} |\psi_s(\vec{x})|^2$$

$$= 1 ,$$

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

$$= 1 , \text{ and}$$

$$|e^{i\phi_s(\vec{x})}|^2 = \frac{|\psi_s(\vec{s})|}{|\psi_s(\vec{x})|}$$

$$= 1 .$$

The latter gives $\phi_s(\vec{x}) \in [0, 2\pi]$.
With these definitions we obtain:

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

$$= \psi_s(\vec{x}) .$$

This in turn gives the desired result:

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

$$= \int_{\mathcal{R}} d\vec{x} f(\vec{x}) |\vec{x}\rangle \sum_s e^{i\phi_s(\vec{x})} \sqrt{p_s(\vec{x})} |s\rangle$$

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