Probability current and thermodynamics of open quantum systems

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This paper explores the generalization of the concept of a “probability current”, familiar from wave-function quantum mechanics, to quantum systems with finite-dimensional Hilbert spaces. The generalized definition applies both to isolated systems evolving via the Schrödinger equation and to more general open systems obeying the Lindblad master equation. We establish several properties of the probability current and explore its relation to thermodynamic heat and work.

I. INTRODUCTION

Consider a quantum system described by a Hilbert space $\mathcal{H}$ of finite dimension $d$. A non-degenerate observable is described by an orthonormal basis $\{ |n\rangle \}$ for $\mathcal{H}$, each basis vector associated with a measurement outcome. If the system state vector is $|\psi\rangle$ then the probability of the $n$th basis state is

$$P_n = |\langle n |\psi\rangle|^2.$$  

As the system state evolves, this probability changes, but the total probability remains 1. That is, probability is “conserved”.

We can express this idea by defining a probability current $J_{nm}$, which is interpreted as the net rate at which probability “flows” from state $m$ to state $n$. The probability current $J_{nm}$ is real and antisymmetric—that is, $J_{nm} = -J_{nm}$. (As a corollary, $J_{nn} = 0$ for any basis state $n$.) The net rate of change of $P_n$ will be given by

$$\frac{dP_n}{dt} = \dot{P}_n = \sum_m J_{mn}.$$  

Such probability flows are familiar from classical master equations [1]. There, $P_n$ represents the classical probability that a system is in state $n$, and $W_{mn}$ represents the conditional rate at which the system jumps from state $m$ to state $n$. Then

$$\dot{P}_n = \sum_m (W_{nm} P_m - W_{mn} P_n).$$  

For this sort of system, the classical probability current $J_{nm} = W_{nm} P_m - W_{mn} P_n$ is real and antisymmetric, and Equation 3 is exactly Equation 2.

Quantum probabilities do not change according to a classical master equation, but rather are governed by the underlying dynamics of the quantum state. For an informationally isolated system [2], the state vector $|\psi\rangle$ evolves according to the Schrödinger equation

$$|\psi\rangle = i \frac{d}{dt} |\psi\rangle,$$  

where $H$ is the system’s Hamiltonian operator. (Here, and in all subsequent expressions, we have set $\hbar = 1$.) To make later generalizations more natural, we re-express Equation 4 in terms of the density operator $\rho$, which for a pure state is the projection $|\psi\rangle\langle\psi|$ onto the state vector:

$$\dot{\rho} = \frac{d\rho}{dt} = \frac{1}{i} [H, \rho].$$  

This equation of motion also applies to mixed states of the system, for which $\rho$ is a positive trace-1 operator rather than a projection. In any case, the probability $P_n = \langle n |\rho |n\rangle = \rho_{nn}$.

Silva [3] derived a probability current $J_{nm}$ between basis states for a system evolving according to Equation 5, applying his result to a one-dimensional model of electron transport. More recently, Roden and Whaley [4] have presented a generalization that applies to open-system dynamics, in which the density operator obeys a master equation of a particular Lindblad type. They use this to analyze how energy flows between complexes of states, with particular attention to energy transport in molecular processes such as photosynthesis.

The main purpose of this paper is to define a general probability current $J_{nm}$ for an evolving quantum system. For Schrödinger evolution, we will show the close connection between our definition and the familiar probability current density $\dot{J}$ of wave-function quantum mechanics. We also show how to extend our definition to arbitrary Lindblad evolution, and we note several important characteristics of the current $J_{nm}$, including its invariance...
under the choice of Lindblad representation. We then use the probability current to characterize the rates of thermodynamic work and heat for a quantum system exchanging energy with its environment.

II. SCHRÖDINGER EVOLUTION

Suppose the state $\rho$ of a quantum system evolves according to Equation (5) and let $\{|n\rangle\}$ be a fixed orthonormal basis for $\mathcal{H}$. To define a suitable probability current $J_{nm}$, we begin with the time rate of change of $P_n = \langle n | \rho | n \rangle$:

$$
\dot{P}_n = \langle n | \dot{\rho} | n \rangle = \frac{i}{\hbar} \langle n | (H - \mu \mathcal{J}) | n \rangle = \frac{1}{\hbar} \sum_m \left( \langle n | H | m \rangle \langle m | \rho | n \rangle - \langle n | \rho | m \rangle \langle m | H | n \rangle \right) - \frac{1}{\hbar} \langle n | \rho | m \rangle \langle m | H | n \rangle \tag{6}
$$

This motivates us to define

$$
J_{nm} = \frac{1}{\hbar} (H_{nm} \rho_{mn} - \rho_{nm} H_{mn}). \tag{7}
$$

Since $H$ and $\rho$ are both Hermitian, $H_{nm} = H_{nm}$ and $\rho_{nm} = \rho_{mn}$. Thus, $J_{nm}$ is both real and antisymmetric, and it automatically satisfies Equation (4).

Under what conditions can $J_{nm}$ be nonzero? Equation (4) gives us important necessary conditions. First of all, the Hamiltonian operator must have a nonzero matrix element $H_{nm}$. This is a restatement of the well-known fact that transitions between basis states are produced by the off-diagonal elements of $H$.

Less familiar is the corresponding condition on $\rho$: $J_{nm} \neq 0$ only if the coherence $\rho_{nm} \neq 0$. This means that, for example, in an incoherent mixture of $|n\rangle$ and $|m\rangle$ states, the probability current $J_{nm} = 0$. Furthermore, the positivity of $\rho$ implies that

$$
|\rho_{nm}|^2 = |\rho_{nm}|^2 = P_n P_m. \tag{8}
$$

Thus, $J_{nm} \neq 0$ only if both $P_n > 0$ and $P_m > 0$. This is the basis for the “quantum Zeno effect” [3]. If $P_n = 0$ at any moment, then it is also true that

$$
\dot{P}_n = \sum_m J_{nm} = 0. \tag{9}
$$

For Schrödinger evolution, therefore, the departure of $P_n$ from 0 cannot be linear in time. Repeated measurements of the $\{|n\rangle\}$ basis constantly reset $P_n = 0$ and thus suppress transitions to this state.

The idea of a “probability flow” is a familiar one from the quantum mechanics of particles moving in one or more continuous spatial dimensions. Consider a particle of mass $\mu$ moving in one dimension. The wave function $\Psi$ yields a probability density $P = |\Psi|^2$ for the outcome of a hypothetical position measurement. We define a probability current density by

$$
J = \frac{1}{2\mu} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right). \tag{10}
$$

If the particle moves subject to a potential $U(x)$, its wave function evolves according to the Schrödinger equation

$$
- \frac{1}{2\mu} \frac{\partial^2 \Psi}{\partial x^2} + U(x) \Psi = i \frac{\partial \Psi}{\partial t}. \tag{11}
$$

Then the probability density satisfies a continuity equation

$$
\frac{\partial P}{\partial t} = - \frac{\partial J}{\partial x}. \tag{12}
$$

These results are easily generalized to 3-D, in which the probability current density is a vector $\vec{J}$.

How is our probability current related to these standard definitions? We replace the continuous spatial coordinate $x$ with a discrete lattice of points $x_n$, with adjacent points separated by $\Delta x$. In the state $|n\rangle$, the particle is localized to the nth lattice point. These localized states form an orthonormal basis for the Hilbert space, so we can write any state as

$$
|\psi\rangle = \sum_n \psi_n |n\rangle, \tag{13}
$$

where $\psi_n = \langle n | \psi \rangle$. We define the wave function $\Psi(x_n) = \psi_n / \sqrt{\Delta x}$, so that

$$
\sum_n |\psi_n|^2 = \sum_n |\Psi(x_n)|^2 \Delta x \rightarrow \int |\Psi(x)|^2 \, dx \tag{14}
$$

in the continuous ($\Delta x \rightarrow 0$) limit. A lattice approximation to the left-hand side of Equation (11) tells us how the Hamiltonian operator $H$ affects the amplitudes of the state $|\psi\rangle$:

$$
\langle n | H | \psi \rangle = - \frac{1}{2\mu} \left( \psi_{n+1} - 2\psi_n + \psi_{n-1} \right) - U(x_n) \psi_n. \tag{15}
$$

Therefore, the Hamiltonian matrix elements are

$$
H_{nm} = - \frac{1}{2\mu} \left( \psi_{n+1,m} - 2\delta_{nm} + \psi_{n-1,m} \right) + U(x_n) \delta_{nm}. \tag{16}
$$

For the pure state $|\psi\rangle$ the matrix elements of the density operator are $\rho_{nm} = \psi_n \psi^*_m$.

From Equation (16) we can see that the only non-zero probability currents $J_{nm}$ are those for which $n$ and $m$ are adjacent lattice sites. The net rightward probability
current between sites \( n \) and \( n+1 \) is
\[
J_{n+1,n} = \frac{1}{\Delta x} \left( H_{n+1,n} \psi_n \psi_n^* + \psi_{n+1} \psi_n^* H_{n,n+1} \right)
\]
\[
= -\frac{1}{2 \mu i \Delta x} \left[ (\psi_n \psi_n^* - \psi_{n+1} \psi_n^*) (\psi_n \psi_n^* - \psi_{n+1} \psi_n^*) \right]
\]
\[
= -\frac{1}{2 \mu i \Delta x} \left[ \Psi(x_n) \Psi^*(x_{n+1}) - \Psi(x_{n+1}) \Psi(x_n)^* \right].
\]
Given the lattice approximation for the derivative at \( x_n \)
\[
\frac{\partial \Psi}{\partial x} = \frac{\Psi(x_{n+1}) - \Psi(x_n)}{\Delta x},
\]
we obtain
\[
J_{n+1,n} = -\frac{1}{2 \mu i} \left[ \Psi(x_n) \left( \Psi^*(x_n) + \frac{\partial \Psi^*}{\partial x} \Delta x \right) \right.
\]
\[
- \Psi^*(x_n) \left( \Psi(x_n) + \frac{\partial \Psi}{\partial x} \Delta x \right) \right]
\]
\[
= \frac{1}{2 \mu i} \left( \Psi \frac{\partial \Psi}{\partial x} - \Psi^* \frac{\partial \Psi^*}{\partial x} \right),
\]
where the wave functions and derivatives are evaluated at \( x_n \). This is exactly the lattice approximation for \( J(x_n) \) as defined in Equation 10 above.

The probability density \( P(x_n) = |\Psi(x_n)|^2 = P_n / \Delta x \), so its time derivative is
\[
\frac{\partial P}{\partial t} = \frac{\dot{P}_n}{\Delta x} = J_{n,n+1} + J_{n-1,n}
\]
\[
= J(x_n) - J(x_{n-1}) / \Delta x,
\]
which yields Equation 12 as \( \Delta x \to 0 \). Thus, our discrete probability current \( J_{nm} \) between sites of the lattice reduces to the conventional probability current density in the continuous limit.

III. LINDBLAD SYSTEMS

An open quantum system can exchange energy and information with its environment, leading to correlations between system and environment. However, it may happen that these correlations are rapidly “hidden” in distant or inaccessible parts of the environment, so that on intermediate timescales the system and environment remain effectively uncorrelated. Under these circumstances, the time evolution of the quantum system is approximately Markovian and may be described by a quantum master equation known as the Lindblad equation [2]:
\[
\dot{\rho} = \frac{1}{i \hbar} [H, \rho] + \sum_{\alpha} \left( L_\alpha \rho L_\alpha^\dagger - \frac{1}{2} \{ L_\alpha^\dagger L_\alpha, \rho \} \right),
\]
where \( \{ \cdots, \cdots \} \) is the anticommutator. The \( L_\alpha \) operators represent interactions with the environment that lead to non-unitary evolution for \( \rho \). (The Hamiltonian \( H \) may also include effects from these interactions.) It is sometimes convenient to write Equation 21 in a more compact form
\[
\dot{\rho} = \frac{1}{i \hbar} [H, \rho] + \mathcal{L}(\rho),
\]
where \( \mathcal{L} \) is the map defined by the Lindblad operators \( L_\alpha \).

The additional terms in Equation 21 require us to generalize the definition of the probability current \( J_{nm} \). The simplest approach is as follows. We first rewrite \( \mathcal{L} \) in a more symmetrical form:
\[
\mathcal{L}(\rho) = \frac{1}{3} \sum_{\alpha} \left( L_\alpha \rho L_\alpha^\dagger - L_\alpha^\dagger L_\alpha \rho - \rho L_\alpha^\dagger L_\alpha \right).
\]
We now fix a basis and calculate \( \dot{P}_n = \langle n | \dot{\rho} | n \rangle \). The Hamiltonian term produces a “Hamiltonian current” exactly as before. Additional terms due to the \( \mathcal{L}(\rho) \) map can be found by introducing a complete basis \( \{|m\} \) at appropriate points within the operator products. This procedure yields
\[
J_{nm} = J_{nm}^{(H)} + \sum_{\alpha} J_{nm}^{(\alpha)}
\]

where \( J_{nm}^{(H)} \) is the Hamiltonian current defined previously in Equation 7 and
\[
J_{nm}^{(\alpha)} = \frac{1}{2} \left( (L_\alpha \rho)L_{nm}^\dagger + L_{nm}^\dagger (L_\alpha \rho) \right.
\]
\[
- (L_\alpha^\dagger \rho)L_{nm} \right)
\]
represents the contribution to the probability current produced by a single Lindblad operator \( L_\alpha \).

We can readily verify that \( J_{nm} \) is real and antisymmetric, and that the Lindblad equation guarantees that Equation 2 holds.

Note that our probability current is a linear functional of the state \( \rho \). This is a reasonable property for \( J_{nm} \). Suppose the density operator \( \rho \) is a probabilistic mixture of two states: \( \rho = p_1 \rho_1 + p_2 \rho_2 \). Then all probabilities are also mixtures:
\[
P_n = p_1 \langle n | \rho_1 | n \rangle + p_2 \langle n | \rho_2 | n \rangle.
\]
It thus makes sense that the probability currents \( J_{nm} \), which are related to the rates of change \( \dot{P}_n \), behave in the same way under mixtures:
\[
J_{nm} = p_1 J_{nm,1} + p_2 J_{nm,2},
\]
as Equation 24 implies.

The representation of open system evolution in Equation 21 is not unique. Suppose we replace the \( L_\alpha \) operators with modified \( M_\beta \) operators, where
\[
M_\beta = \sum_{\alpha} U_{\beta \alpha} L_\alpha,
\]
and the $U_{\beta\alpha}$ coefficients are the elements of a unitary matrix. The resulting Lindblad equation is exactly equivalent to the original. To see this, we first note that

$$\sum_{\beta} U_{\beta\alpha}^* U_{\beta\gamma} = \sum_{\beta} (U^\dagger)_{\alpha\beta} U_{\beta\gamma} = \delta_{\alpha\gamma}. \quad (29)$$

Using this it is not hard to verify that

$$\sum_{\beta} M_{\beta\gamma}^* M_{\beta\alpha} = \sum_{\alpha} L_{\alpha}^* L_{\alpha},$$

$$\sum_{\beta} M_{\beta\gamma}^* \rho M_{\beta\alpha} = \sum_{\alpha} L_{\alpha}^* \rho L_{\alpha} \quad (30)$$

Therefore the open system dynamics described by Equation 24 will be unchanged by the replacement of the $L$-operators with $M$-operators. The two sets of operators, \{L_{\alpha}\} and \{M_{\beta}\}, are sometimes called two unravelings of the same Lindblad master equation.

The definition of $J_{nm}$ in Equation 24 has the same general structure as the Lindblad equation itself. Each term involving $L_{\alpha}$ also involves $L_{\alpha}^*$, and the index $\alpha$ is summed over. Therefore, the value of the probability current $J_{nm}$ is independent of our choice of unravelling of the master equation. The individual $J_{nm}$ terms, of course, may be different for different unravelings, but their sum will be the same.

IV. A FLOW PARADOX

Consider a system governed by a classical master equation. Equation 3 with classical probability current $J_{nm} = W_{nm} P_m - W_{mn} P_n$. If both $P_n = 0$ and $P_m = 0$, the current $J_{nm}$ from $m$ to $n$ must be zero as well. If only $P_n = 0$, we can still have a nonzero $J_{nm}$; however, since the conditional rates $W_{mn} \geq 0$ for all pairs of states, we can conclude that $J_{nm} \geq 0$ in this case. If a state $n$ has zero probability, the net flow of probability between $n$ and some other state $m$ can only be directed toward $n$.

By contrast, for a quantum system governed by the Schrödinger equation (Equation 5), the quantum probability flow $J_{nm} = 0$ if either $P_n = 0$ or $P_m = 0$.

What about the generalized definition of $J_{nm}$ for Lindblad evolution (Equation 24)? Consider a qubit system $Q$ with basis states $|0\rangle$ and $|1\rangle$, whose dynamics may be described by a single Lindblad operator $L = \sqrt{\lambda} |0\rangle \langle 1|$, where $\lambda$ is a constant. (This might describe a decay process in a two level atom from the excited state $|1\rangle$ to the ground state $|0\rangle$.) If at a particular moment the state $\rho$ is described by the density operator $\rho = |1\rangle \langle 1|$, the probability current $J_{01} = \lambda$ (and so $\dot{P}_0 = \lambda$), even though $\rho_0 = 0$.

This fact presents us with a puzzle. We may consider a composite system comprising $Q$ and its environment $E$. The complete system $QE$ is informationally isolated, so that the evolution of its joint state is described by the Schrödinger equation. If we choose basis states $\{|a\rangle\}$ for $Q$ and $\{|b\rangle\}$ for $E$, the joint probability is $P_{ab}$, and the total probability for $Q$-state $n$ is

$$P_n = \sum_a P_{na}. \quad (31)$$

Thus, if $P_n = 0$, then it must be that all of the probabilities $P_{na} = 0$. From this it follows that all probability currents $J_{na,mb} = 0$ in this composite system.

What is the relation between $J_{na,mb}$ for $QE$ and $J_{nm}$ for $Q$ alone? This can be seen by considering how $P_n$ is changing over time:

$$\dot{P}_n = \sum_a \dot{P}_{na} = \sum_a \left( \sum_{mb} J_{na,mb} \right)$$

$$= \sum_m \left( \sum_{ab} J_{na,mb} \right). \quad (32)$$

Hence we identify

$$J_{nm} = \sum_{ab} J_{na,mb}. \quad (33)$$

We may conclude that, if $P_n = 0$ for the subsystem $Q$, the rate of change $\dot{P}_n = 0$ too.

However, as our decaying qubit example shows, this is not necessarily true for evolution described by the Lindblad equation. We may have $P_n = 0$ but $J_{nm}$ and $\dot{P}_n$ both nonzero. How can this behavior arise if the global state is evolving unitarily?

The answer comes from recognizing that the Lindblad equation can only be an approximation to the exact evolution of a subsystem state. Consider another system, an isolated qubit with internal Hamiltonian

$$H = -\omega Y = i\omega (|0\rangle \langle 1| - |1\rangle \langle 0|). \quad (34)$$

The state of the system happens to be the pure state $|\psi\rangle = \epsilon |0\rangle + \sqrt{1 - \epsilon^2} |1\rangle$, where $\epsilon \ll 1$. Then

$$\rho = |\psi\rangle \langle \psi| = \epsilon^2 |0\rangle \langle 0| + \epsilon \sqrt{1 - \epsilon^2} |0\rangle \langle 1| + \sqrt{1 - \epsilon^2} |1\rangle \langle 0| + (1 - \epsilon^2) |1\rangle \langle 1| \quad (35)$$

The probability $P_0 = \rho_{00} = \epsilon^2$. The probability current is

$$J_{01} = \frac{1}{i} (H_{01} \rho_{10} - \rho_{01} H_{10}) = 2\omega \epsilon \sqrt{1 - \epsilon^2}. \quad (36)$$

To lowest order in $\epsilon$, $J_{01} \approx 2\omega \epsilon$. Thus, if we consider an approximation in which we keep $O(\epsilon)$ terms but discard $O(\epsilon^2)$ terms, we will say that $P_0 = 0$ but $J_{01} \neq 0$ in our approximation.

Suppose therefore that the environment $E$ has a Hilbert space of large dimension $D$. (Such a complex environment would be required in order to continually “hide” its correlations with $Q$.) For a given system state $Q$, we can consider a state for which the $|n,a\rangle$ basis states...
have small (that is, $O(\epsilon)$) amplitudes. Then $P_{na} \sim \epsilon^2$ for each $a$, and thus
\[ P_n = \sum_a P_{na} \sim D\epsilon^2. \] (37)

On the other hand, we may expect $J_{na,mb} \sim \epsilon$, and so
\[ J_{nm} = \sum_{ab} J_{na,mb} \sim D^2\epsilon. \] (38)

If $\epsilon$ is small and $D$ is large, it may be that $D\epsilon^2$ is negligible, but $D^2\epsilon$ is finite. This is why the approximate Lindblad evolution can have $P_n = 0$ but $J_{nm} \neq 0$.

In this way, Lindblad evolution behaves more like a classical master equation. On the other hand, the quantum case can exhibit some distinctly non-classical features. Consider a system with dimension $n$, and the non-unitary part of the evolution is given by a single Lindblad operator
\[ L = \sqrt{\lambda} (|3\rangle \langle 1| - 2|2\rangle \langle 3|). \] (39)

(That is, the only non-zero matrix elements are $L_{31} = 1$ and $L_{32} = -2$.) Our state $\rho = |\psi\rangle \langle \psi|$, where $|\psi\rangle = \frac{1}{\sqrt{3}} (|1\rangle + |2\rangle)$. From this we can calculate that $P_3 = \rho_{33} = 0$ and
\[ J_{31} = -\frac{\lambda}{4} \text{ and } J_{32} = +\frac{\lambda}{2}. \] (40)

Not only are these non-zero, but $J_{13} = -J_{31}$ (the net probability current from state 3 to state 1) is actually positive. We may have a positive probability current from a state of zero probability! (No actual paradox is involved, since $J_{31} + J_{32} > 0$, so the net probability current is into the zero-probability state 3.)

In spite of this surprising situation, it remains true that if both $P_n$ and $P_m$ are zero, the current $J_{nm} = 0$ also, even for Lindblad evolution. The simplest way to prove this is to note that if $P_n = \rho_{nn} = 0$, then $\rho_{nk} = \rho_{kn} = 0$ for all $k$, and thus for any $L$
\[ (\rho L)_{nm} = \sum_k \rho_{nk} L_{km} = 0 \quad \text{and} \quad (L\rho)_{mn} = \sum_k L_{mk} \rho_{kn} = 0. \] (41)

Each term in Equation (35) involves a factor of this type, and so $J_{nm}^{(a)} = 0$ for every Lindblad operator $L_a$. (The Hamiltonian part of the current $J_{nm}^{(H)} = 0$ as well, by the arguments given above.)

V. HEAT AND AND PROBABILITY FLOW

The Hamiltonian $H$ is the energy operator for a system, and the system’s mean energy is the expectation
\[ \langle E \rangle = \text{Tr} \rho H. \] (42)
The value of $\langle E \rangle$ can change in two distinct ways. The system state $\rho$ may change, or the Hamiltonian $H$ may change due to the modification of one or more external parameters (e.g., a change in an externally applied magnetic field). Thus, we may write
\[ \frac{d}{dt} \langle E \rangle = \text{Tr} \dot{\rho} H + \text{Tr} \rho \dot{H}. \] (43)

These two terms correspond to thermodynamic heat and work, respectively. That is, if we let $P_Q$ and $P_W$ denote the rates at which heat and work are transferred to the system, we may write
\[ P_Q = \text{Tr} \dot{\rho} H \quad \text{and} \quad P_W = \text{Tr} \rho \dot{H}. \] (44)

Consider a system interacting with its environment so that its evolution is described by the Lindblad equation (Equation 22). Note that the Hamiltonian $H$ and the Lindblad operators $L_a$ may depend on time. We find that
\[ P_Q = \text{Tr} \dot{\rho} H = \text{Tr} \left( \frac{i}{\hbar} [H, \rho] \right) H + \text{Tr} L(\rho) H = \frac{1}{i} \text{Tr} (H \rho H - \rho H^2) + \text{Tr} L(\rho) H = \text{Tr} L(\rho) H, \] (45)
since $\text{Tr} H \rho H = \text{Tr} \rho H H$. Only the non-unitary part of the dynamics described by the map $L$ affects the heat rate $P_Q$. This map is absent if the system is informationally isolated, so $P_Q = 0$. Thus, energy changes in such a system can only involve work done on the system, not heat transfer to the system.

In this section and the next, we will explore the relation of $P_Q$ and $P_W$ to the probability current $J_{nm}$. For our basis we choose the energy eigenbasis, in which the eigenstate $|n\rangle$ has energy $E_n$ and the Hamiltonian operator is diagonal:
\[ H = \sum_n E_n |n\rangle \langle n|. \] (46)

This has the advantage that the Hamiltonian part of the current $J_{nm}^{(H)} = 0$. It has the disadvantage that the Hamiltonian may vary with time. Thus, $P_n$ and $J_{nm}$ will be defined with respect to a basis $\{|n\rangle\}$ that is not fixed, but itself has some time-dependence. As we will see below, this requires us to introduce additional terms in some of our expressions.

Heat transfer, however, can be analyzed with the expressions already in hand, simply by adopting the instantaneous energy eigenbasis $\{|n\rangle\}$ and defining $J_{nm}$...
according to Equation 24. We obtain

\[ \mathcal{P}_Q = \sum_n E_n \langle n | \mathcal{L}(\rho) | n \rangle \]

\[ = \sum_n \sum_\alpha E_n \left( (L_\alpha \rho L_\alpha^\dagger)_{nn} - \frac{i}{2} (L_\alpha^\dagger L_\alpha \rho - \frac{1}{2} (\rho L_\alpha^\dagger L_\alpha)_{nn}) \right) \]

\[ = \sum_{nm} \sum_\alpha E_{nm} J^{(\alpha)}_{nm} \]

(47)

where the \( J^{(\alpha)}_{nm} \) currents are defined in Equation 25. Since the Hamiltonian current \( J^{(H)}_{nm} = 0 \), we may simply write

\[ \mathcal{P}_Q = \sum_{nm} E_{nm} J_{nm}. \]

(48)

By reindexing the last sum, we note that

\[ \sum_{nm} E_{nm} J_{nm} = \sum_{nm} E_{m} J_{mn} = - \sum_{nm} E_{m} J_{nm}. \]

(49)

Therefore we may write

\[ \mathcal{P}_Q = \frac{1}{2} \sum_{nm} (E_n - E_m) J_{nm}. \]

(50)

If the eigenbasis \( \{|n\rangle\} \) of the Hamiltonian is time-independent, the interpretation of Equation 50 is straightforward. A transition of the system from state \( m \) to state \( n \) produces a change in system energy \( \Delta E = E_n - E_m \). The current \( J_{nm} \), is, in a probabilistic sense, the net rate at which such transitions are happening. The factor of \( 1/2 \) arises because the double sum counts each distinct pair of states twice. We could in fact rewrite Equation 50 as

\[ \mathcal{P}_Q = \sum_{n,m} E_{nm} J_{nm}. \]

(51)

We can also write Equation 50 as

\[ \mathcal{P}_Q = \sum_\alpha \left( \frac{1}{2} \sum_{nm} (E_n - E_m) J^{(\alpha)}_{nm} \right) = \sum_\alpha \mathcal{P}^{(\alpha)}_Q. \]

(52)

The different Lindblad operators \( L_\alpha \) may represent different physical processes. For example, it may be that our system of interest is interacting with two different parts of the environment—heat baths at different temperatures, perhaps. We may be able to partition the set of Lindblad operators into two groups, one for each external system. By dividing the terms of the sum in Equation 52 we can determine separate heat transfer rates from the two external systems.

VI. WORK AND THE ROTATING EIGENBASIS

Now we turn to the situation in which the Hamiltonian \( H \), which is both the instantaneous energy observable and the generator of the unitary part of the time evolution in Equation 21, can itself vary over time. We write

\[ \dot{H} = \frac{d}{dt} \left( \sum_n E_n \langle n | \langle n \rangle \right) \]

\[ = \sum_{nm} \dot{E}_n \langle n | \langle n \rangle + \sum_{nm} E_n \left( \frac{d}{dt} \langle n | \langle n \rangle \right). \]

(53)

The first sum yields an operator \( R:\)

\[ R = \sum_{n} \dot{E}_n \langle n | \langle n \rangle. \]

(54)

This operator, which commutes with \( H \), describes how the energy eigenvalues are changing.

How do the basis states \( |n\rangle \) change over time? Since the basis remains orthonormal, the basis vectors must change unitarily. This unitary evolution is generated by a Hermitian operator \( K \), which appears in a “Schrödinger” equation for \( |n(t)\rangle:\)

\[ K |n(t)\rangle = i \frac{d}{dt} |n(t)\rangle, \]

(55)

which can also be written as

\[ \frac{d}{dt} |n\rangle\langle n| = \frac{i}{\hbar} [K, |n\rangle\langle n|]. \]

(56)

This lets us simplify the second sum in Equation 53:

\[ \sum_n E_n \left( \frac{d}{dt} |n\rangle\langle n| \right) = \frac{i}{\hbar} \sum_n \dot{E}_n [K, |n\rangle\langle n|] \]

\[ = \frac{i}{\hbar} [K, H]. \]

(57)

Therefore we can write

\[ \dot{H} = R + \frac{1}{i\hbar} [K, H], \]

(58)

where the operators \( R \) and \( K \) describe the changes in the eigenvalues and eigenstates of \( H \), respectively.

How does the change in basis—a change in our “reference frame” in the Hilbert space—affect probability currents? At any moment, the probability of the \( n \)-th state is \( P_n = \langle n | \rho | n \rangle \), as before; but now both \( \rho \) and \( |n\rangle \) may be changing:

\[ \dot{P}_n = \langle n | \dot{\rho} | n \rangle + \frac{1}{i\hbar} \text{Tr} \rho [K, |n\rangle\langle n|]. \]

(59)

1 We are assuming that both the eigenvalues and eigenstates of \( H \) vary in a smooth and continuous way. This is not necessarily true for the eigenstates. Consider a qubit with \( H(t) = \alpha t^2 \mathbb{Z} \) for \( t \leq 0 \) and \( H = \alpha t^2 X \) for \( t > 0 \). At \( t = 0 \), \( H \) is well-defined (and equals zero), but the eigenbasis for \( H \) changes instantaneously from the \( Z \)-basis to the \( X \) basis. This can happen because the energy eigenvalues are degenerate at \( t = 0 \). Any small perturbation to \( H \) that lifts this degeneracy will also remove the discontinuity. Since the discontinuous case relies on a special exact degeneracy, we adopt the assumptions of Equation 58 as physically reasonable in the generic case.
By cyclically permuting terms in the trace, we can transform this to
\[ \dot{P}_n = \langle n | \left( \dot{\rho} - \frac{1}{i} [K, \rho] \right) | n \rangle. \]  
(60)

As far as the changes in \( P_n \) are concerned, the effect of the change in basis is the same as introducing a new term \(-K\) into the Hamiltonian. Thus, we introduce a frame current
\[ I_{nm} = -\frac{1}{i} (K_{nm} \rho_{nm} - \rho_{nm} K_{mn}), \]  
(61)

and write
\[ \dot{P}_n = \sum_m (J_{nm} + I_{nm}). \]  
(62)

The probability currents \( J_{nm} \) are related to changes in the quantum state \( \rho \) and are defined as in Equations (24) and (23). To account for all changes in probability, including those produced by our shifting basis, we need to include the frame current \( I_{nm} \) as well.

The rate at which work is done on the system is
\[ P_W = \text{Tr} \rho H = \text{Tr} \rho R + \frac{1}{i} \text{Tr} \rho [K, H] = \text{Tr} \rho R - \frac{1}{i} \text{Tr} \rho [K, \rho] H. \]  
(63)

In the energy eigenbasis this becomes
\[ P_W = \sum_n P_n \dot{E}_n + \sum_{nm} E_n I_{nm}. \]  
(64)

Using the antisymmetry of the frame current \( I_{nm} \), we obtain
\[ P_W = \sum_n P_n \dot{E}_n + \frac{1}{2} \sum_{nm} (E_n - E_m) I_{nm}. \]  
(65)

The second term in Equation (65) resembles the heat transfer rate in Equation (50) but it involves the frame current \( I_{nm} \) rather than \( J_{nm} \). It tells us that work can be done on a quantum system either by shifting the energy levels (the \( \dot{E}_n \) term) or by rotating the energy basis. Consider a spin in an external magnetic field. We may do work on the spin either by changing the magnitude of the field (which changes the energy eigenvalues) or by rotating the field to a new spatial direction (which changes the energy eigenstates).

To summarize, we have found that the mean energy of the system changes by
\[ \frac{d}{dt} \langle E \rangle = \left( \frac{\mathcal{P}_Q}{\mathcal{P}_W} \right) \left( \sum_{nm} (E_n - E_m) J_{nm} \right) + \left( \sum_n P_n \dot{E}_n + \frac{1}{2} \sum_{nm} (E_n - E_m) I_{nm} \right). \]  
(66)

where \( \mathcal{P}_Q \) and \( \mathcal{P}_W \) are the rates of heat and work energy transfers to the system.

VII. REMARKS

We have proposed particular definitions for the probability current \( J_{nm} \). For informationally isolated systems evolving according to the Schrödinger equation, the definition in Equation (7) suffices; for systems evolving via a Lindblad master equation, we have the more general definition in Equation (23). These definitions share a number of general properties:

- \( J_{nm} \) is real.
- \( J_{nm} \) is antisymmetric in \( n \) and \( m \).
- Given a fixed basis set \( \{ |n\rangle \} \), \( \dot{P}_n = \sum m J_{nm} \).
- \( J_{nm} \) is independent of the particular unraveling of the quantum master equation via Lindblad operators.
- \( J_{nm} \) is a linear functional of the state \( \rho \).

We must note, however, that these properties are shared by many other definitions. Suppose \( a_{nm} \) is an arbitrary real antisymmetric matrix of coefficients such that every row sums to zero, and let \( B \) be a Hermitian operator. Then the revised expression
\[ J'_{nm} = J_{nm} + a_{nm} (\text{Tr} \rho B) \]  
(67)

yields probability currents that satisfy all of the general properties we have listed.

A similar ambiguity exists for the probability current density \( \vec{J} \) for a particle moving in three dimensions. Together with the probability density \( \mathcal{P} = |\Psi|^2 \), the current density satisfies the continuity equation:
\[ \frac{\partial \mathcal{P}}{\partial t} = -\nabla \cdot \vec{J}. \]  
(68)

If we define a new current density \( \vec{J}' = \vec{J} + \vec{K} \), where \( \nabla \cdot \vec{K} = 0 \), the continuity equation for probability is still satisfied.

In fact, many of our results work equally well for the modified probability current of Equation (67). Consider the heat rate relation from Equation (48). If we replace \( J_{nm} \) by \( J'_{nm} \), we obtain
\[ \sum_{nm} E_n J'_{nm} = \sum_{nm} E_n J_{nm} + \sum_{nm} E_n a_{nm} (\text{Tr} \rho B) \]
\[ = \mathcal{P}_Q + \sum_n E_n (\text{Tr} \rho B) \left( \sum_m a_{nm} \right) = \mathcal{P}_Q. \]  
(69)

The modified currents are related to heat transfer in exactly the same way as before.

Since the definitions in Equation (7) and (23) are so closely connected to the dynamical equations, we believe that they are the simplest choices for the probability currents.
They also have some reasonable properties that are not shared by some of the alternatives given by Equation [67]. For instance, under our definitions, if $P_n$ and $P_m$ are both zero, then $J_{nm} = 0$; but it is easy to come up with examples for which $J'_{nm} \neq 0$. This raises an unresolved question: Can we devise a reasonable, physically motivated set of general properties for the probability currents $J_{nm}$ that uniquely determine their definition?

In spite of the apparent arbitrariness of the definitions given here, we anticipate that the probability currents $J_{nm}$ will be a useful tool for understanding the dynamics of quantum systems with finite-dimensional Hilbert spaces. The connections between probability currents and thermodynamic work and heat also suggest that they will be helpful in analyzing the function of quantum thermodynamic systems like the small thermal machines analyzed in [6].

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