Conserved current in Markovian open-quantum systems

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We reexamine the Markovian approximation of local current in open quantum systems, discussed recently by Gebauer and Car. Our derivation is more transparent; the proof of the current conservation becomes explicit and easy.

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I. INTRODUCTION

Quantum mechanics is reversible at the microscopic level. If, however, an atomic system is coupled to a reservoir, then the atomic reduced dynamics becomes irreversible and the corresponding evolution equation contains a memory term. Yet, in the Markov approximation the time evolution of the atomic reduced density matrix $\hat{\rho}$ satisfies the memory less master equation:

$$\frac{d\hat{\rho}}{dt} = -i[\hat{H},\hat{\rho}] + \mathcal{L}\hat{\rho}, \tag{1}$$

where $\hat{H}$ is the atomic Hamiltonian. The irreversible term can be written into the Lindblad form [1,2]:

$$\mathcal{L}\hat{\rho} = \sum_i (\hat{V}_i^\dagger \hat{\rho} \hat{V}_i - \hat{V}_i \hat{V}_i^\dagger \hat{\rho}) g_i + \text{H.c.}, \tag{2}$$

where $\{\hat{V}_i\}$ are certain atomic operators and $\{g_i\}$ are complex coefficients satisfying $\text{Re}\, g_i > 0$. This equation constitutes the phenomenological dynamics of the given Markovian open quantum system.

In Hamiltonian dynamics with *local* potentials and interactions, an important conserved quantity is the particle density. Consider, for simplicity sake, a single atomic electron with the canonical pair of operators $\hat{\mathbf{x}}, \hat{\mathbf{p}}$. The electron's density operator at location $\mathbf{r}$ reads as

$$\hat{n}(\mathbf{r}) = \delta(\mathbf{r} - \hat{\mathbf{x}}) = |\mathbf{r}\rangle\langle\mathbf{r}|, \tag{3}$$

where the position eigenstates satisfy the equation $\hat{\mathbf{x}}|\mathbf{r}\rangle = \mathbf{r}|\mathbf{r}\rangle$. There is a local current defined by

$$\hat{\mathbf{J}}(\mathbf{r}) = \frac{1}{2m}[\hat{\mathbf{p}}\hat{n}(\mathbf{r}) + \hat{n}(\mathbf{r})\hat{\mathbf{p}}]. \tag{4}$$

The current $\hat{\mathbf{J}}$ is conserved, i.e., the Heisenberg operators $\hat{n}_t, \hat{\mathbf{J}}_t$ satisfy the continuity equation:

$$\frac{d\hat{n}_t(\mathbf{r})}{dt} + \nabla \cdot \hat{\mathbf{J}}_t(\mathbf{r}) = 0. \tag{5}$$

A similar continuity equation follows for the expectation values as well. The continuity equation still holds if the atom interacts with other systems, provided the interaction is *local*. Let us, indeed, suppose a certain local interaction with a reservoir. The atom becomes an open system governed by the master equation (1) in the Markovian approximation. Let us write down the continuity equation for the expectation values of $\hat{n}$ and $\hat{\mathbf{J}}$ in the atomic state $\hat{\rho}$, and substitute Eq. (1). In the Schrödinger picture we obtain the following:

$$\frac{d\langle\hat{n}(\mathbf{r})\rangle}{dt} + \nabla \cdot \langle\hat{\mathbf{J}}(\mathbf{r})\rangle = \langle\mathcal{L}^*\hat{n}(\mathbf{r})\rangle. \tag{6}$$

We see that the extra term $\langle\mathcal{L}^*\hat{n}(\mathbf{r})\rangle \equiv \text{tr}[\hat{n}(\mathbf{r})\mathcal{L}\hat{\rho}]$ on the rhs may in general violate the local conservation of the current. Gebauer and Car [3] noticed that such a violation is a consequence of the Markov approximation. They also pointed out that current conservation can be restored by adding a dissipative correction $\hat{\mathbf{J}}_D$ to the Hamiltonian current $\hat{\mathbf{J}}$. These authors have derived $\hat{\mathbf{J}}_D$ from the exact reversible dynamics of the atom+reservoir. Here we reconsider the issue and propose a shorter and transparent derivation. Our formulating $\hat{\mathbf{J}}_D$ is fairly explicit to satisfy local conservation. This latter is the main progress with respect to Ref. [3], which would need a subtle and lengthier proof [4], not even published in Ref. [3] or elsewhere.

It is clear from Eq. (6) that $\hat{\mathbf{J}} + \hat{\mathbf{J}}_D$ will satisfy the continuity equation if:

$$\nabla \cdot \hat{\mathbf{J}}_D(\mathbf{r}) = -\mathcal{L}^*\hat{n}(\mathbf{r}). \tag{7}$$

In one dimension with boundary conditions $\hat{\mathbf{J}}_D(\pm\infty) = 0$, the previous equation has a unique solution $\hat{\mathbf{J}}_D(r) = -\int_{-\infty}^{r} dr'\, \mathcal{L}^*\hat{n}(r')$, but in higher dimensions, additional considerations are necessary to uniquely determine $\hat{\mathbf{J}}_D$. In fact, the Markov dynamics (1) of the atomic state $\hat{\rho}$ is not sufficient to calculate $\hat{\mathbf{J}}_D$. We must carefully inspect the Markov approximation of the exact current. In Sec. II we review the derivation of the master equation (1) in the usual Born-

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Markov approximation. Then Sec. III ontains our derivation of the dissipative current $\hat{\mathbf{J}}_D$.

II. BORN-MARKOV APPROXIMATION

Let $\hat{H}+\hat{K}+\hat{H}_R$ stand for the total Hamiltonian, where $\hat{H}$ belongs to the atomic system, and $\hat{H}_R$ belongs to the reservoir. The interaction Hamiltonian is local; we consider the simple case $\hat{K}=\hat{V}(\hat{\mathbf{x}})\hat{F}$, where the "field" $\hat{F}$ is a reservoir operator [5]. We suppose that the initial state of the whole system is $\hat{\rho}\hat{\rho}_R$, where $\hat{\rho}_R$ is the reservoir equilibrium state. We denote by $\hat{O}_\tau$ the operator $\hat{O}$ at time τ in the interaction picture. Let us introduce the reservoir correlation function,

$$g(\sigma-\tau)=\mathrm{tr}_R(\hat{F}_\sigma\hat{F}_\tau\hat{\rho}_R), \tag{8}$$

which is a complex non-negative time-translation invariant kernel. Consider the change of the atomic reduced density matrix during a certain time Δ. In the interaction picture, second order perturbation theory yields

$$\frac{\hat{\rho}_\Delta-\hat{\rho}}{\Delta}=\frac{1}{\Delta}\int_0^\Delta d\sigma\int_0^\sigma d\tau(\hat{V}_\tau\hat{\rho}\hat{V}_\sigma-\hat{V}_\sigma\hat{V}_\tau\hat{\rho})g(\sigma-\tau)+\mathrm{H.c.}, \tag{9}$$

where the first order term in $\hat{V}$ vanishes since we assume $\mathrm{tr}_R(\hat{F}\hat{\rho}_R)=0$. Suppose that $\tau_A\gg\tau_R$, where τ_A is the time scale of atomic state evolution and τ_R is the reservoir correlation time. Choose Δ in between the reservoir and atomic time scales:

$$\tau_R\ll\Delta\ll\tau_A. \tag{10}$$

A standard way to proceed is the Born-Markov approximation that requires weak coupling and results in the master equation (1) for the atomic state $\hat{\rho}_t$ *time-coarse grained on scale* Δ.

The implementation of the Born-Markov approximation has two steps. We identify the lhs of (9) by the time derivative $d\hat{\rho}/dt$ of the time-coarse-grained atomic state $\hat{\rho}$. On the rhs, we extend the integration limit as well as the denominator Δ to ∞. The latter limit is rigorously justified by a particular rescaling [6] where $\hat{V}\to 0$, while $\hat{V}^2\Delta$ is constant [7]. Accordingly, the explicit form of the Lindblad-superoperator becomes

$$\mathcal{L}\hat{\rho}=\lim_{t\to\infty}\frac{1}{t}\int_0^t d\sigma\int_0^\sigma d\tau(\hat{V}_\tau\hat{\rho}\hat{V}_\sigma-\hat{V}_\sigma\hat{V}_\tau\hat{\rho})g(\sigma-\tau)+\mathrm{H.c.} \tag{11}$$

It is easy to inspect that the rhs is already of the Lindblad form (2). To achieve the familiar spectral representation, we expand the interaction potentials as

$$\hat{V}_\tau=\sum_\omega e^{i\omega\tau}\hat{V}_\omega, \tag{12}$$

where the sum is over all possible transition frequencies $\omega=\epsilon_n-\epsilon_m$ of the system Hamiltonian $\hat{H}=\Sigma_n\epsilon_n|n\rangle\langle n|$. Obviously, the spectral component of $\hat{V}$ is of this form,

$$\hat{V}_\omega=\hat{V}_{-\omega}^\dagger=\sum_{\substack{n,m\\ \epsilon_n-\epsilon_m=\omega}}|n\rangle V_{nm}\langle m|. \tag{13}$$

As $t\to\infty$, the oscillating terms in the integral (11) drop out, and we get the master equation (1) where

$$\mathcal{L}\hat{\rho}=\sum_\omega(\hat{V}_\omega^\dagger\hat{\rho}\hat{V}_\omega-\hat{V}_\omega\hat{V}_\omega^\dagger\hat{\rho})g_\omega^{(+)}+\mathrm{H.c.}, \tag{14}$$

and

$$g_\omega^{(+)}=\int_0^\infty d\tau\, e^{i\omega\tau}g(\tau). \tag{15}$$

III. THE MARKOVIAN CONSERVED CURRENT

Constructing the correct Markovian coarse-grained current, $\hat{\mathbf{J}}+\hat{\mathbf{J}}_D$ needs special care. First, we calculate the average of the exact current over the period Δ of time-coarse graining. We expect that it becomes the sum of the unperturbed contribution $\hat{\mathbf{J}}$ and the Markovian correction $\hat{\mathbf{J}}_D$ in the Born-Markov limit,

$$\frac{1}{\Delta}\int_0^\Delta d\sigma\langle\hat{\mathbf{J}}\rangle_\sigma\to\langle\hat{\mathbf{J}}\rangle+\langle\hat{\mathbf{J}}_D\rangle, \tag{16}$$

where $\langle\ldots\rangle_\sigma$ stands for the expectation value in the exact time-dependent state evolved from $\hat{\rho}\hat{\rho}_R$ by the total Hamiltonian $\hat{H}+\hat{H}_R+\hat{K}$ while $\langle\ldots\rangle$ stands for the expectation value in the coarse-grained state $\hat{\rho}$. Let us introduce the time-dependent auxiliary variable $\hat{\mathbf{Z}}(\mathbf{r};t)$, defined as

$$\hat{\mathbf{Z}}(\mathbf{r};t)=\int_0^t d\sigma\,\hat{\mathbf{J}}_\sigma(\mathbf{r}). \tag{17}$$

Then, in the interaction picture, the lhs of (16) can be written as

$$\frac{1}{\Delta}\mathrm{tr}\,\hat{\mathbf{Z}}(\Delta)\hat{\rho}_\Delta-\frac{1}{\Delta}\mathrm{tr}\int_0^\Delta d\sigma\,\hat{\mathbf{Z}}(\sigma)\frac{d\hat{\rho}_\sigma}{d\sigma}. \tag{18}$$

In the Born-Markov limit, the time-coarse-grained atomic state $\hat{\rho}_t$ evolves smoothly and only "differentially" during time Δ, so does the current $\hat{\mathbf{J}}_\sigma$, too, in such states: we can thus write the first term as just $\langle\hat{\mathbf{J}}\rangle$. In the second term, *before taking the Born-Markov limit*, we substitute the perturbative expression of $d\hat{\rho}_\sigma/d\sigma$:

$$-\frac{1}{\Delta}\mathrm{tr}\int_0^\Delta d\sigma\,\hat{\mathbf{Z}}(\sigma)\int_0^\sigma d\tau(\hat{V}_\tau\hat{\rho}\hat{V}_\sigma-\hat{V}_\sigma\hat{V}_\tau\hat{\rho})g(\sigma-\tau)+\mathrm{H.c.} \tag{19}$$

Now we take the Born-Markov limit, which, again, allows us to calculate the rhs by taking the limit $\Delta\to\infty$:

$$\langle \hat{\mathbf{J}}_D \rangle = -\lim_{t\to\infty} \frac{1}{t} \mathrm{tr} \int_0^t d\sigma \int_0^\sigma d\tau\, \hat{\mathbf{Z}}(\sigma)(\hat{V}_\tau \hat{\rho} \hat{V}_\sigma - \hat{V}_\sigma \hat{V}_\tau \hat{\rho}) g(\sigma - \tau) + \mathrm{H.c.} \tag{20}$$

We can express the dissipative current itself,

$$\hat{\mathbf{J}}_D = -\lim_{t\to\infty} \frac{1}{t} \int_0^t d\sigma \int_0^\sigma d\tau [\hat{V}_\sigma \hat{\mathbf{Z}}(\sigma) \hat{V}_\tau - \hat{\mathbf{Z}}(\sigma) \hat{V}_\sigma \hat{V}_\tau] g(\sigma - \tau) + \mathrm{H.c.} \tag{21}$$

Recall that $\hat{\mathbf{Z}}(\mathbf{r};\sigma) = \int_0^\sigma d\lambda\, \hat{\mathbf{J}}_\lambda(\mathbf{r})$, so that $\hat{\mathbf{J}}_D(\mathbf{r})$ has turned out to be a local linear functional of the unperturbed local current $\hat{\mathbf{J}}(\mathbf{r})$.

It is easy to prove that $\hat{\mathbf{J}}_D$ contributes properly to current conservation. Let us take the divergence of both sides of Eq. (21). Observe that

$$\boldsymbol{\nabla} \cdot \hat{\mathbf{Z}}(\sigma) = -\hat{n}_\sigma + \hat{n}, \tag{22}$$

because density conservation $\nabla \hat{\mathbf{J}}_\sigma + d\hat{n}_\sigma / d\sigma = 0$ holds for the unperturbed atomic current and density. We have assumed that the interaction is local, so $[\hat{n}_\sigma, \hat{V}_\sigma] = 0$. Therefore the terms proportional to $\hat{n}_\sigma$ cancel each other on the rhs of Eq. (21), and we obtain

$$\boldsymbol{\nabla} \cdot \hat{\mathbf{J}}_D = -\lim_{t\to\infty} \frac{1}{t} \int_0^t d\sigma \int_0^\sigma d\tau (\hat{V}_\sigma \hat{n} \hat{V}_\tau - \hat{n} \hat{V}_\sigma \hat{V}_\tau) g(\sigma - \tau) + \mathrm{H.c.} \tag{23}$$

The rhs coincides with $-\mathcal{L}^* \hat{n}$ as it should; cf. Eq. (7).

IV. CLOSING REMARKS

Our central result is the expression (21) of the dissipative current $\hat{\mathbf{J}}_D$. Its form was convenient when we proved the continuity equation from the locality of the interaction. In concrete calculations, however, the spectral representation is the preferred one. As the spectral representation of $\hat{\mathbf{Z}}(\sigma)$ is

$$\hat{\mathbf{Z}}(\sigma) = \sum_{\omega_J} \hat{\mathbf{J}}_{\omega_J} \frac{e^{i\omega_J \sigma} - 1}{i\omega_J}, \tag{24}$$

Eq. (21) yields two terms for the spectral expression of $\hat{\mathbf{J}}_D$. To compare it with the result of Car and Gebauer [3], we present the spectral expression of the expectation value:

$$\langle \hat{\mathbf{J}}_D \rangle = \mathrm{tr} \left(\sum_{\substack{\omega_J + \omega_1 - \omega_2 = 0 \\ \omega_\rho = 0}} - \sum_{\substack{\omega_1 - \omega_2 = 0 \\ \omega_J + \omega_\rho = 0}} \right) \frac{\hat{\mathbf{J}}_{\omega_J}}{i\omega_J} (\hat{V}^\dagger_{\omega_2} \hat{\rho}_{\omega_\rho} \hat{V}_{\omega_1} - \hat{V}_{\omega_1} \hat{V}^\dagger_{\omega_2} \hat{\rho}_{\omega_\rho}) g^{(+)}_{\omega_2} + \mathrm{H.c.} \tag{25}$$

Here $\hat{\mathbf{J}}_{\omega_J}$, $\hat{\rho}_{\omega_\rho}$, and $\hat{V}_\omega$ are the respective spectral representations of $\hat{\mathbf{J}}$, $\hat{\rho}$ and $\hat{V}$; cf. Eq. (13). The two sums cancel the singularity at $\omega_J = 0$. We note without going into detail that, for nondegenerate transition frequencies, our result (25) coincides with Eq. (16) in [3], apart from minor typos of the latter [8].

Our result allows us to calculate the Markovian correction $\hat{\mathbf{J}}_D$ to the local current in open quantum systems with a discrete spectrum. The method applies to quantum dots directly [9]. The case of quantum Brownian motion, however, requires a suitably modified approach to cope with the Markovian limit of an open system with a continuous spectrum.

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[5] The generic form of $\hat{K}$ is $\hat{V}_1(\hat{\mathbf{x}})\hat{F}_1 + \hat{V}_2(\hat{\mathbf{x}})\hat{F}_2 + \ldots$, and our results can immediately be extended to such general interactions.
[6] Temporarily, rewrite the interaction Hamiltonian into the form $\lambda \hat{K}$, where λ is the parameter of coupling. In the limit $\lambda \to 0$, the second-order perturbative expression yields the exact time-derivative of the coarse-grained atomic state $\hat{\rho}$ for times of order λ^{-2} [7]. Accordingly, the rhs of Eq. (9) can equivalently be calculated if we make the subsitutions $\hat{K} \to \lambda \hat{K}$ and $\Delta \to \lambda^{-2}\Delta$ at $\lambda \to 0$. This is equivalent with the limit indicated on the rhs of Eq. (11).
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[8] For the reader's convenience, let us match the structure and notations of Eq. (25) with those of [3]. The first and the second sums of the rhs are related to $\mathcal{T}_{kl}$ and $\mathcal{R}_{kl}$ in [3]. In our notations, $\mathcal{T}_{kl} = \Sigma^{\omega_1 - \omega_2 = \epsilon_k - \epsilon_l}_{\omega_\rho = 0} (\hat{V}^\dagger_{\omega_2} \hat{\rho}_{\omega_\rho} \hat{V}_{\omega_1} - \hat{V}_{\omega_1} \hat{V}^\dagger_{\omega_2} \hat{\rho}_{\omega_\rho}) g^{(+)}_{\omega_2} + \mathrm{H.c.}$ In the correct version of [3], $\mathcal{T}_{kl} = \Sigma_{n \neq k} [\hat{V}_{kn} \bar{S}_{nn}(t) \hat{V}_{nl} w^+_{nk} - \hat{V}_{kn} \hat{V}_{nl} \bar{S}_{ll}(t) w^+_{ln}] + \mathrm{H.c.}$ Concerning $\mathcal{R}_{kl}$ we note that if there are no transition frequency degeneracies then $\hat{V}^\dagger_{\omega_1} \hat{\rho}_{\omega_\rho} \hat{V}_{\omega_1}$ has nonvanishing terms only if $\omega_\rho = 0$. So the sandwich term drops out and that is why $\mathcal{R}_{kl}$ in [3] has only two terms.
[9] In preparation.