Quantum master equation for a system of charged fermions interacting with the electromagnetic field

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Abstract

A quantum master equation with microscopic coefficients is proposed to describe the dissipative dynamics of a Fermi system coupled with an environment of particles through a two-body potential. In comparison with other master equations existing in literature, this equation satisfies the conditions of a dynamical detailed balance, leading to Pauli master equations for the diagonal elements of the density matrix, and to damped Bloch-Feynman equations for the non-diagonal ones during the whole evolution of the system. The new equation is particularized for a harmonic oscillator coupled with the electromagnetic field through electric-dipole interaction and is compared with the well-known equation of Sandulescu and Scutaru.

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Quantum master equations represent an essential tool for describing the interplay between dissipative and field-induced processes in a matter-field system. Recently, vivid discutions have been devoted to this subject [1–12], but generally acccepting that the dissipative dynamics of an N-level system is correctly described by a time-dependent semigroup of evolution operators [13–16]. These operators satisfy Lindblad's master equation [14]

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}[H,\rho(t)] + \frac{1}{2\hbar}\sum_{n=1}^{N^2-1}([V_n\rho(t),V_n^+] + [V_n,\rho(t)V_n^+]) \tag{1}$$

that, depending on the linear combinations

$$V_n = \sum_m a_{nm}s_m \tag{2}$$

of the system operators s_m, is valid only for a weak dissipative coupling. In comparison with other master equations taking into account a strong dissipative coupling [17,18], it has the advantage of entirely preserving the quantum-mechanical properties of the density matrix (hermiticity, trace-class and positivity) during the whole evolution of the system. However, Eq. (1) is only a general form with $(N^2-1)^2$ free complex parameters for an N-level system that has only N^2-1 degrees of freedom. General conditions for describing the dynamics of a physical system in accordance with the detailed balance principle have recently been derived [2]. The connection of this axiomatic equation with the previous phenomenological descriptions has been realized by Sandulescu and Scutaru [19]. Thus, for a unidimensional system with the coordinate x and the momentum p, one may define the dissipative operators

$$V_n = a_n p + b_n x \tag{3}$$

that lead to a quantum master equation

$$\begin{aligned}\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}[H,\rho(t)] - \frac{i\lambda}{2\hbar}([x,p\rho(t)+\rho(t)p] - [p,x\rho(t)+\rho(t)x]) - \\ -\frac{D_{pp}}{\hbar^2}[x,[x,\rho(t)]] - \frac{D_{xx}}{\hbar^2}[p,[p,\rho(t)]] + \\ +\frac{D_{px}}{\hbar^2}([x,[p,\rho(t)]] + [p,[x,\rho(t)]])\end{aligned} \tag{4}$$

with a friction coefficient

$$\lambda = \sum_{n=1}^{2}\frac{a_n^* b_n - a_n b_n^*}{2i}, \tag{5}$$

and three diffusion coefficients

$$D_{xx} = \frac{\hbar}{2}\sum_{n=1}^{2}a_n^* a_n, \quad D_{pp} = \frac{\hbar}{2}\sum_{n=1}^{2}b_n^* b_n, \quad D_{px} = -\frac{\hbar}{2}\sum_{n=1}^{2}\frac{a_n^* b_n + a_n b_n^*}{2}. \tag{6}$$

¿From these expressions, one obtains fundamental constraints of the dissipative coefficients:

$$D_{pp} > 0, \quad D_{qq} > 0, \quad D_{pp}D_{qq} - D_{pq}^2 > \frac{\hbar^2\lambda^2}{4}. \tag{7}$$

It is remarkable that Eq. (4), originally obtained only from the condition of the probability normalization [14], satisfies also Heisenberg's uncertainty relation $\Delta x \cdot \Delta p \geq \hbar/2$ during the whole evolution of the system [19]. It is suggested that for Eq. (4), originally derived for deep inelastic processes (heavy-ion collisions), any values of the friction/diffusion coefficients satisfying the relations (7) are in principle allowed. Some interesting effects of quantum optics [20] and nuclear physics [21–23], predicted in this framework, have experimental evidence.

Considering an equilibrium asymptotic solution according to Boltzmann's distribution, for a harmonic oscillator with the frequency ω_0 this equation takes a form

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}[H,\rho(t)] - \frac{\gamma}{4\hbar}\left\{ (Font) LaTeX Font Warning : Command invalid in math mode 1214.5ptc \right. \quad \text{co} \tag{8}$$

depending only on two parameters: the decay rate $\gamma = 2\lambda$ and temperature T. It is also remarkable that this equation, derived only from the asymptotic condition, satisfies also the condition of a detailed balance during the whole evolution of the system. Really, from (8), one obtains equations for matrix elements

$$\begin{aligned}\frac{d}{dt}\rho_{mn}(t) = -i(m-n)\omega_0\rho_{mn}(t) - \frac{\gamma}{2}\Big\{ & \left[(m+n+1)\coth\left(\frac{\hbar\omega_0}{2T}\right) - 1\right]\rho_{mn}(t) - \\ & -\sqrt{(m+1)(n+1)}\left[\coth\left(\frac{\hbar\omega_0}{2T}\right)+1\right]\rho_{m+1,n+1}(t) - \\ & -\sqrt{mn}\left[\coth\left(\frac{\hbar\omega_0}{2T}\right)-1\right]\rho_{m-1,n-1}(t)\Big\}\end{aligned} \tag{9}$$

that, for the diagonal ones, take a form

$$\begin{aligned}\frac{d}{dt}\rho_{nn}(t) = \frac{\gamma}{2}\Big\{(n+1)&\left[\left(\coth\frac{\hbar\omega_0}{2T}+1\right)\rho_{n+1,n+1}(t) - \left(\coth\frac{\hbar\omega_0}{2T}-1\right)\rho_{nn}(t)\right] + \\ +n&\left[\left(\coth\frac{\hbar\omega_0}{2T}-1\right)\rho_{n-1,n-1}(t) - \left(\coth\frac{\hbar\omega_0}{2T}+1\right)\rho_{nn}(t)\right]\Big\}\end{aligned} \tag{10}$$

with an asymptotic solution corresponding to Boltzmann's distribution

$$\frac{\rho_{n+1,n+1}(\infty)}{\rho_{nn}(\infty)} = \frac{\rho_{nn}(\infty)}{\rho_{n-1,n-1}(\infty)} = e^{-\frac{\hbar\omega_0}{T}}. \tag{11}$$

We notice that, according to this equation, the population variation of an arbitrary level n is the result of the population transitions from the two neighbouring levels $n+1, n-1$. This corresponds to a dipole coupling of the harmonic oscillator: only the dipole moments of a harmonic oscilator have the property of being non-zero only between two successive levels. Really, the master equation (8) has beeen reobtained for a harmonic oscillator coupled with the electromagnetic field in an independent oscillator model [24], that corresponds to an electric-dipole interaction - the field variation with the oscillator coordinate is not taken into account.

However, although Eqs. (10) are in agreement with a principle of detailed balance in a sense recently discussed [2–4], Eqs. (9) for the non-diagonal matrix elements describe non-physical couplings of a transition $m \leftrightarrow n$ with the neighbouring transitions $m-1 \leftrightarrow n-1$ and $m+1 \leftrightarrow n+1$. The possibility of such couplings is discuused in [25], as representing a coherence transfer between equidistant levels - in this case, all the transitions between equidistant levels should be coupled. This is not the case here, where the couplings of the transitions between the neighbouring levels appear merely by using Lindblad's master equation with only two operators x and p - these couplings are present for an arbitrary unidimensional potential [26,19]: the derivation of Eq. (4) is exclusively based on the general relations (3), without any additional assumption about the potential. Here the essential problem is that one may not expect to describe precisely the dynamics of an N-level system with only two operators x and p, even though this system has the simpler form of a harmonic oscillator.

This description with only two operators has been used to obtain a master equation in agreement with the quantum-mechanical principles, without increasing too much the number of the free parameters introduced through Lindblad's axiomatic formalism [19]. However, as it was previously shown by Ford, Lewis and O'Connell [3,24], the preservation of the quantum-mechanical conditions is possible also in a constructive approach [27], where the dissipative parameters can be effectively calculated. Thus, for a system of fermions with the creation-destruction operators $c_i^+ \; - \; c_i$ and the Hamiltonian H, one obtains a master equation of the form [28–30]

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar}[H,\rho(t)] + \sum_{ij} \lambda_{ij}([c_i^+ c_j \rho(t), c_j^+ c_i] + [c_i^+ c_j, \rho(t) c_j^+ c_i]), \tag{12}$$

depending on $N^2 - 1$ coefficients with the expressions

$$\lambda_{ij} = \lambda_{ij}^F = \frac{\pi}{\hbar Y^F} \int |\langle \alpha i | V^F | \beta j \rangle|^2 [1 - f_\alpha^F(\varepsilon_\alpha)] f_\beta^F(\varepsilon_\beta) g_\alpha^F(\varepsilon_\alpha) g_\beta^F(\varepsilon_\beta) d\varepsilon_\beta, \quad \varepsilon_{\alpha\beta} = \varepsilon_{ji} \tag{13}$$

for a dissipative environment of Y^F fermions, and

$$\lambda_{ij} = \lambda_{ij}^B = \frac{\pi}{\hbar Y^B} \int |\langle \alpha i | V^B | \beta j \rangle|^2 [1 + f_\alpha^B(\varepsilon_\alpha)] f_\beta^B(\varepsilon_\beta) g_\alpha^B(\varepsilon_\alpha) g_\beta^B(\varepsilon_\beta) d\varepsilon_\beta, \quad \varepsilon_{\alpha\beta} = \varepsilon_{ji} \tag{14}$$

for a dissipative environment of Y^B bosons. In this expressions, V^F, V^B are dissipative two-body potentials, $g_\alpha^F(\varepsilon_\alpha), g_\beta^F(\varepsilon_\beta), g_\alpha^B(\varepsilon_\alpha), g_\beta^B(\varepsilon_\beta)$ are densities of the environment states, and $f_\alpha^F(\varepsilon_\alpha), f_\beta^F(\varepsilon_\beta), f_\alpha^B(\varepsilon_\alpha), f_\beta^B(\varepsilon_\beta)$ are occupation probabilities of these states. In this description, a transition $|j\rangle \to |i\rangle$ of a system particle is correlated with a transition $|\beta\rangle \to |\alpha\rangle$ of an environment particle. When the environment is a blackbody electromagnetic field coupled with the system through a dipole moment $\vec{r}_{ij}$, we obtain the dissipative coefficients [30]:

$$\lambda_{ij} = \gamma_{ij} = \frac{2\alpha_0}{c^2\hbar^3} \vec{r}_{ij}^{\,2} \varepsilon_{ji}^3 (1 + \frac{1}{e^{\varepsilon_{ji}/T} - 1}) \equiv \mu_{ij}[1 + f_\alpha^B(\varepsilon_{ji})], \tag{15}$$

where $\alpha_0 = \frac{e^2}{4\pi\varepsilon_0 \hbar c} \approx \frac{1}{137}$.

¿From the quantum master equation (12) one obtains equations of matrix elements

$$\frac{d}{dt}\rho_{mn}(t) = -i\omega_{mn}\rho_{mn}(t) + \sum_j [2\delta_{mn}\lambda_{mj}\rho_{jj}(t) - (\lambda_{jm} + \lambda_{jn})\rho_{mn}(t)] \tag{16}$$

that, for the diagonal matrix elements, lead to master equations of Pauli's form

$$\frac{d}{dt}\rho_{nn}(t) = 2\sum_j [\lambda_{nj}\rho_{jj}(t) - \lambda_{jn}\rho_{nn}(t)], \tag{17}$$

and, for the non-diagonal matrix elements, take the form of the damped Bloch-Feynman equations [31]

$$\frac{d}{dt}\rho_{mn}(t) = -i\omega_{mn}\rho_{mn}(t) - \Lambda_{mn}\rho_{mn}(t) \tag{18}$$

with dephasing rates

$$\Lambda_{mn} = \sum_j (\lambda_{jm} + \lambda_{jn}). \tag{19}$$

We notice that Eqs. (18) do not contain any dissipative couplings between different transition elements as $\rho_{mn}(t)$ with $\rho_{m-1,n-1}(t)$ or $\rho_{m+1,n+1}(t)$), such as Eqs. (9) do. Such couplings are not revealed in the most studies of quantum optics [31–35].

With the matrix elements

$$x_{n-1,n} = x_{n,n-1} = \sqrt{\frac{n\hbar}{2M\omega_0}}, \tag{20}$$

the quantum master equation (12) with the coefficients (15) can particularized for a harmonic oscillator in a blackbody radiation field

$$\begin{aligned} \frac{d}{dt}\rho(t) =& -\frac{i}{\hbar}[H,\rho(t)] + \\ +\alpha_0\frac{\hbar\omega_0^2}{Mc^2}\sum_n\Big\{&\frac{n+1}{e^{\hbar\omega_0/T}-1}([c_{n+1}^+c_n\rho(t),c_n^+c_{n+1}] + [c_{n+1}^+c_n,\rho(t)c_n^+c_{n+1}]) + \\ &+n\left(1+\frac{1}{e^{\hbar\omega_0/T}-1}\right)([c_{n-1}^+c_n\rho(t),c_n^+c_{n-1}] + [c_{n-1}^+c_n,\rho(t)c_n^+c_{n-1}])\Big\} \end{aligned} \tag{21}$$

In comparison with Eq. (8), the new equation (21) describes transitions between any two successive levels of a harmonic oscillator with dipole coupling and, besides, parametrically depends only on temperature. The corresponding Bloch equations

$$\begin{aligned} \frac{d}{dt}\rho_{mn}(t) = -i(m-n)\omega_0\rho_{mn}(t) - \alpha_0\frac{\hbar\omega_0^2}{Mc^2}\Big\{&\left[(m+n+1)\coth\left(\frac{\hbar\omega_0}{2T}\right)-1\right]\rho_{mn}(t) - \\ &-\delta_{mn}(n+1)\left[\coth\left(\frac{\hbar\omega_0}{2T}\right)+1\right]\rho_{m+1,n+1}(t) - \\ &-\delta_{mn}n\left[\coth\left(\frac{\hbar\omega_0}{2T}\right)-1\right]\rho_{m-1,n-1}(t)\Big\} \end{aligned} \tag{22}$$

take the same form as (9) only for the diagonal matrix elements, while for the non-diagonal matrix elements the couplings of $\rho_{mn}(t)$ with $\rho_{m-1,n-1}(t)$ and $\rho_{m+1,n+1}(t)$ are no more present. In this formalism, couplings of the transitions between the equidistant levels of a harmonic oscillator [25] could be taken into account only as higher-order terms in the weak-coupling expansion of the dissipative dynamics [24].

As a conclusion, we have obtained a quantum master equation with transition operators $c_i^+ c_j$, and microscopic coefficients depending on matrix elements, densities of the environment states, and occupation probabilities of these states. This equation describes the dynamics of an N-level system of fermions in agreement with the principle of a dynamical detailed balance: (1) Pauli master equations for populations, (2) damped Bloch-Feynman equations for polarizations.

We discussed this equation in the context of other master equations describing the time-evolution of a system ia accordance with the quantum-mechanical principles. For a harmonic oscillator coupled with the electromagnetic field, we obtained a master equation with $N-1$ transition operators between successive levels. Although the old equation in x and p satisfies the detailed balance condition (1) for the diagonal matrix elements, it fails for the non-diagonal matrix elements, including non-physical couplings between these elements. These couplings appear as an approximation effect, due to the utilization of only two operators x and p for the N^2-1 operators of an N-level system. The operators x and p, simultaneously including all the transition operators, do not enable the separation of the most probable resonant particle-particle couplings.

In this approach, we obtained a master equation in the second-order approximation that, describing single-particle transitions, is valid only for a weak dissipative coupling. A stronger dissipative coupling can be taken into acount in a higher-order approximation, describing correlated transitions of fermions.

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