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Microscopic treatment of energy dissipation and decoherence via many-body Lindblad superoperators

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Abstract. Starting from a recent reformulation of the Markov limit, we apply the mean-field approximation to the resulting Lindblad-type many-electron dynamics, and derive a closed equation of motion for the electronic single-particle density matrix in the presence of one- and two-body scattering mechanisms. The proposed formulation preserves the positive-definite character of the single-particle density matrix. This result is in striking contrast with conventional Markov approaches, where the single-particle mean-field equations can lead to positivity violations and therefore to unphysical results.

One of the most challenging problems in the microscopic modeling of state-of-the-art electronic quantum systems and devices is the derivation of suitable scattering superoperators (see, e.g., [1]) to account for decoherence and dissipation phenomena (see, e.g., [2, 3, 4]). When the system-environment coupling becomes strong and/or the excitation timescale is extremely short, Markovian approaches are known to be unreliable, and memory effects have to be taken into account via quantum-kinetic approaches (see, e.g., [5, 6]); however, even in regimes where the Markov limit is applicable, conventional Markov approaches may lead to unphysical results, such as negative eigenvalues of the density matrix. To overcome this serious limitation, a few years ago an alternative and more general Markov procedure has been proposed [7]; however, in spite of its conceptual importance, the practical implementation of the latter is limited by the fact that the many-body evolution is in general not exactly solvable. So far, all relevant applications of such Markov treatment to semiconductor nanosystems are limited to the low-density limit, where a Lindblad-type scattering-induced evolution is demonstrated also for the single-particle density matrix (see, e.g., [8, 9]).

Aim of this contribution is to discuss a recently proposed kinetic treatment based on a nonlinear density-matrix equation [10]. More specifically, by applying the conventional mean-field approximation to the many-electron dynamics obtained via the alternative Markov limit recalled above, it is possible to derive a closed equation of motion for the electronic single-particle density matrix, in the presence of carrier-carrier as well as carrier-phonon scattering mechanisms. While in the low-density limit such nonlinear equation exhibits a Lindblad form –like for the many-body density matrix– at finite or high carrier concentrations the equation turns out to be non-Lindblad and highly nonlinear. Nevertheless, we can prove that the mean-field approximation does preserve the positive-definite character of the single-particle density matrix, an essential prerequisite of any reliable kinetic treatment of semiconductor quantum

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devices. This result is in striking contrast with the case of mean-field approximations applied to conventional (non-Lindblad) Markov approaches, where the corresponding single-particle equations may lead to positivity violations. The power and flexibility of the proposed density-matrix formalism has been confirmed by a recent investigation of phonon-induced quantum diffusion in state-of-the-art carbon nanotubes [11], where non-linear effects are found to play a relevant role.

The study of electro-optical processes in semiconductors mainly relies on physical quantities that depend on the electronic-subsystem coordinates only. This suggests the introduction of a many-electron density-matrix operator $\hat{\boldsymbol{\rho}}$, defined as the trace of the global (i.e., electron plus various crystal excitations) density-matrix operator over non-relevant degrees of freedom (e.g., phonons, plasmons, etc.). Starting from the alternative Markov procedure proposed in Ref. [7], which allows one to derive a global Lindblad scattering superoperator, it is possible to show that also such a reduced many-electron dynamics is still of Lindblad type, i.e.,

$$\left.\frac{d\hat{\boldsymbol{\rho}}}{dt}\right|_{\text{scat}} = \sum_s \left(\hat{\mathbf{A}}^s \hat{\boldsymbol{\rho}} \hat{\mathbf{A}}^{s\dagger} - \frac{1}{2} \left\{ \hat{\mathbf{A}}^{s\dagger} \hat{\mathbf{A}}^s, \hat{\boldsymbol{\rho}} \right\} \right) , \tag{1}$$

where the explicit form of the reduced or electronic operators $\hat{\mathbf{A}}^s$ can be derived starting from the global Lindblad ones.

Within the above description, one has already performed a statistical average over the phonon bath, but the electronic subsystem is still treated via a many-body picture. However, in the investigation of semiconductor-based quantum materials and devices, many of the physical observables of interest (like, e.g., total carrier density, mean kinetic energy, charge current, and so on) may be well described via single-particle electronic operators. The study of the time evolution of such single-particle quantities requires the derivation of a closed equation of motion for the single-particle density matrix $\rho_{\alpha_1\alpha_2} = \text{tr}\{\hat{c}^\dagger_{\alpha_2}\hat{c}_{\alpha_1}\hat{\boldsymbol{\rho}}\}$. Combining the definition of $\rho_{\alpha_1\alpha_2}$ with the many-electron Lindblad dynamics in Eq. (1), and employing the cyclic property of the trace, one gets:

$$\left.\frac{d\rho_{\alpha_1\alpha_2}}{dt}\right|_{\text{scat}} = \frac{1}{2}\sum_s \text{tr}\left\{ \left[\hat{\mathbf{A}}^{s\dagger}, \hat{c}^\dagger_{\alpha_2}\hat{c}_{\alpha_1} \right] \hat{\mathbf{A}}^s \hat{\boldsymbol{\rho}} \right\} \; + \; \text{H.c.} \tag{2}$$

In order to get a closed equation of motion for the single-particle density matrix, it is now central to specify the form of the many-electron Lindblad operators $\hat{\mathbf{A}}^s$ which, in turn, depends on the particular interaction mechanism considered.

For the case of a generic carrier-phonon (cp) interaction mechanism the corresponding (one-body) Lindblad operator is always of the form

$$\hat{\mathbf{A}}^s = \sum_{\alpha\alpha'} A^{\text{cp}}_{\alpha\alpha'} \hat{c}^\dagger_\alpha \hat{c}_{\alpha'} \; ; \tag{3}$$

the latter describes the phonon-induced carrier transition (i.e., destruction plus creation) from the initial state α' to the final state α. In this case, the label $s \equiv \mathbf{q}, \pm$ shall correspond to the emission $(+)$ or absorption $(-)$ of a phonon with wavevector $\mathbf{q}$.

The Lindblad operator corresponding to carrier-carrier (cc) interaction is of the general (two-body) form

$$\hat{\mathbf{A}}^s = \frac{1}{2} \sum_{\alpha\overline{\alpha},\alpha'\overline{\alpha}'} A^{\text{cc}}_{\alpha\overline{\alpha},\alpha'\overline{\alpha}'} \hat{c}^\dagger_\alpha \hat{c}^\dagger_{\overline{\alpha}} \hat{c}_{\overline{\alpha}'} \hat{c}_{\alpha'} \; ; \tag{4}$$

the latter describes the transition (i.e., destruction plus creation) of our electronic pair from the initial (two-body) state $\alpha'\overline{\alpha}'$ to the final state $\alpha\overline{\alpha}$.

By inserting into Eq. (2) the above written carrier-phonon and carrier-carrier Lindblad operators, and employing the usual fermionic anticommutation relations, one ends up with terms involving average values of four and eight fermionic operators, respectively. At this point, the fundamental step to get a closed equation of motion for the single-particle density matrix consists of performing the well-known mean-field (or correlation-expansion) approximation (see, e.g., [4]). Employing this approximation scheme and omitting renormalization terms [10], the resulting single-particle equation is given by

$$\left.\frac{d\rho_{\alpha_1\alpha_2}}{dt}\right|_{\text{scat}} = \frac{1}{2}\sum_{s}\sum_{\alpha'\alpha'_1\alpha'_2}\left[(\delta_{\alpha_1\alpha'} - \rho_{\alpha_1\alpha'})\,\mathcal{P}^{s}_{\alpha'\alpha_2,\alpha'_1\alpha'_2}\rho_{\alpha'_1\alpha'_2} - (\delta_{\alpha'\alpha'_1} - \rho_{\alpha'\alpha'_1})\mathcal{P}^{s*}_{\alpha'\alpha'_1,\alpha_1\alpha'_2}\rho_{\alpha'_2\alpha_2}\right] + \text{H.c.} \tag{5}$$

with generalized carrier-phonon scattering rates

$$\mathcal{P}^{s=\text{cp}}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2} = A^{\text{cp}}_{\alpha_1\alpha'_1}A^{\text{cp}*}_{\alpha_2\alpha'_2} \tag{6}$$

and generalized carrier-carrier scattering rates

$$\mathcal{P}^{s=\text{cc}}_{\alpha_1\alpha_2,\alpha'_1\alpha'_2} = 2\sum_{\overline{\alpha}_1\overline{\alpha}_2,\overline{\alpha}'_1\overline{\alpha}'_2}(\delta_{\overline{\alpha}_2\overline{\alpha}_1} - \rho_{\overline{\alpha}_2\overline{\alpha}_1})\,\mathcal{A}^{\text{cc}}_{\alpha_1\overline{\alpha}_1,\alpha'_1\overline{\alpha}'_1}\mathcal{A}^{\text{cc}*}_{\alpha_2\overline{\alpha}_2,\alpha'_2\overline{\alpha}'_2}\rho_{\overline{\alpha}'_1\overline{\alpha}'_2}\,, \tag{7}$$

where $\mathcal{A}^{\text{cc}}_{\alpha\overline{\alpha},\alpha'\overline{\alpha}'}$ denotes the totally antisymmetric parts of the two-body coefficients $A^{\text{cc}}_{\alpha\overline{\alpha},\alpha'\overline{\alpha}'}$ in Eq. (4). It is worth noting that, opposite to the generalized carrier-phonon rates in Eq. (6), the generalized carrier-carrier rates in Eq. (7) are themselves a function of the single-particle density matrix; this is a clear fingerprint of the two-body nature of the carrier-carrier interaction.

The crucial issue related to the proposed kinetic treatment is the positivity analysis of the nonlinear density-matrix equation (5). Indeed, if the single-particle density matrix describes a physical state, its eigenvalues are necessarily positive-definite and smaller than one (Pauli exclusion principle); this feature must be preserved during the scattering-induced time evolution. As discussed in detail in Ref. [10], in order to prove that, it is crucial to move from the original single-particle basis $\{|\alpha\rangle\}$ to the time-dependent basis $\{|\lambda\rangle\}$ that instantaneously diagonalizes the single-particle density matrix; more specifically, by denoting with $\Lambda_\lambda = \rho_{\lambda\lambda}$ the generic density-matrix eigenvalue (corresponding to the eigenstate $|\lambda\rangle$), it is possible to show that its time evolution induced by the proposed density-matrix equation (5) is simply given by

$$\frac{d\Lambda_\lambda}{dt} = \sum_{s}\sum_{\lambda'}\left[(1-\Lambda_\lambda)P^{s}_{\lambda\lambda'}\Lambda_{\lambda'} - (1-\Lambda_{\lambda'})P^{s}_{\lambda'\lambda}\Lambda_\lambda\right]\,, \tag{8}$$

where $P^{s}_{\lambda\lambda'} = \mathcal{P}^{s}_{\lambda\lambda,\lambda'\lambda'}$ are positive-definite quantities given by the diagonal elements of the generalized scattering rates [see Eqs. (6) and (7)] written in the instantaneous density-matrix eigenbasis. This result is highly non-trivial: it states that, in spite of the partially coherent nature of the carrier dynamics in (5), the time evolution of the eigenvalues Λ_λ is governed by a non-linear Boltzmann-type equation formally identical to the semiclassical-case one.

We are now in the position to state that the physical interval [0, 1] is the only possible variation range of our eigenvalues Λ_λ; to this end, it is crucial to show that when the latter approach the extremal values, 0 or 1, their time derivatives do not allow them to exit the interval. Indeed, a closer inspection of the Boltzmann-like equation (8) shows that:

(i) if one of the eigenvalues is equal to zero, the corresponding time derivative is always non-negative;

(ii) if one of the eigenvalues is equal to one, its time derivative is always non-positive.

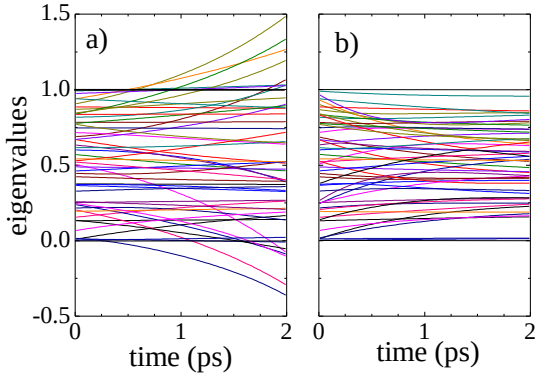

Figure 1. Time evolution of the density matrix eigenvalues, corresponding to a simple two-level system in the presence of carrier-phonon interaction. Panel a): conventional Markov approach; Panel b): proposed single-particle model.

This leads us to the important conclusion that, for both carrier-phonon and carrier-carrier scattering, the proposed nonlinear single-particle equation (5) will preserve the positive-definite character of the single-particle density matrix. We stress that the above positivity analysis is based on the fact that the matrix elements $P^s_{\lambda\lambda'}$ in (8) are positive-definite quantities. This property, which applies to the proposed single-particle equation (obtained starting from the global Lindblad-type scattering superoperator), is generally not fulfilled by conventional Markov models. In this case, starting from a non-Lindblad many-body scattering model, the system dynamics may exit the physical eigenvalue region, giving rise to positivity violations also in the low-density limit [7].

The outcome of the positivity analysis presented so far is fully confirmed by the subset of simulated experiments displayed in Fig. 1, where we report the time evolution of the density-matrix eigenvalues for the case of a simple two-level system, in the presence of carrier-phonon scattering. As expected, for the proposed nonlinear equation all the eigenvalue trajectories fall within the physical interval [0, 1], while for the nonlinear equation obtained within the conventional Markov limit a significant number of simulated eigenvalue trajectories exit the physical interval.

We finally stress that the proposed single-particle formulation has been also extended to the case of quantum systems with spatial open boundaries [10]; this provides a formal derivation of a recently proposed density-matrix treatment based on a Lindblad-like system-reservoir scattering superoperator [8].

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