Microscopic modeling of quantum devices at high carrier densities via Lindblad-like scattering superoperators

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In order to investigate in fully quantum-mechanical terms the electro-optical response of state-of-the-art semiconductor nanomaterials and nanodevices, it is crucial to study the time evolution of single-particle quantities, such as the total carrier density, mean kinetic energy, charge current, and so on. In general, such quantities are given by a suitable (quantum-plus-statistical) average of a corresponding operator, usually expressed in terms of a single-particle density-matrix operator $\hat{\rho}$, whose equation of motion in the low-density limit is always of the form [1]

$$\frac{d\hat{\rho}}{dt} = \frac{1}{i\hbar}\left[\hat{H}_{\rm sp}, \hat{\rho}\right] + \Gamma\left(\hat{\rho}\right) \ , \qquad (1)$$

where $\hat{H}_{\rm sp}$ is the single-particle Hamiltonian and Γ is a linear superoperator describing scattering-induced energy dissipation and decoherence. The degree of accuracy of such density-matrix formalism is intimately related to the choice of the scattering superoperator. Indeed, oversimplified approaches accounting for Γ in a phenomenological way (e.g., T_1T_2 models) or via kinetic treatments based on the conventional Markov limit [2] may lead to the violation of the positive-definite character of the single-particle density-matrix $\hat{\rho}$, and therefore to unphysical results. To overcome this serious limitation, an alternative Markov procedure has recently been proposed [3], showing that in the low-density limit it is possible to microscopically derive a Lindblad-like scattering superoperator of the form

$$\Gamma\left(\hat{\rho}\right) = \sum_s \left(\hat{A}^s\hat{\rho}\hat{A}^{s\dagger} - \frac{1}{2}\left\{\hat{A}^{s\dagger}\hat{A}^s, \hat{\rho}\right\}\right) \ , \qquad (2)$$

thereby preserving the positive-definite character of the single-particle density matrix $\hat{\rho}$. Such formalism has been recently applied to the study of phonon-induced quantum diffusion in GaN-based nanostructures [4].

Primary goal of this contribution is twofold: on the one hand, employing the alternative version of the Markov limit proposed in [3] together with the usual mean-field approximation [5], we shall derive a non-linear (i.e., high-density) version of the scattering superoperator in (2), showing that at finite/high carrier densities the latter is definitely non-Lindblad. On the other hand, we shall propose an approximated version of such high-density scattering superoperator which (i) is still Lindblad-like, and (ii) in the semiclassical limit reduces to the conventional non-linear structure of the Boltzmann collision term.

As a result, the proposed quantum-mechanical generalization of the semiclassical theory in terms of time-dependent Lindblad superoperators will provide a conceptually simple and physically reliable computational framework for the description of various single-particle as well as two-body Coulomb interactions, thus allowing for a predictive (i.e., parameter-free) investigation of new-generation quantum devices over a wide range of operation conditions.

References

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[5] See, e.g., F. Rossi and T. Kuhn, Rev. Mod. Phys. **74**, 895 (2002).

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