Simulation of quantum dot devices by coupling of quantum master equations and semi-classical transport theory

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***Abstract*—We discuss a comprehensive modeling approach for the simulation of quantum dot devices based on the coupling of the van Roosbroeck system with a Markovian quantum master equation. The model equations describe the flow of electrons and holes in semiconductor devices along with a quantum kinetic many-body approach for the quantum dot physics. The consistency of the model equations with respect to non-equilibrium thermodynamics is investigated. We present numerical simulations of an electrically driven single-photon source based on a single quantum dot.**

I. Introduction

Semiconductor quantum dots (QDs) are zero-dimensional nanostructures which provide a (tailorable) discrete spectrum of electronic states due to confinement of charge carriers in all spatial dimensions. Because of their tunable electro-optical properties QDs have attracted considerable attention in particular for applications in solid-state based opto-electronic devices. These include for example highly efficient semiconductor nanolasers with a single or a few QDs as gain medium and quantum light sources such as single-photon emitters and sources of entangled photon pairs. Applications comprise quantum communication and cryptography, on-chip optical computing and quantum information processing.

The modeling and simulation of semiconductor devices containing low-dimensional nanostructures constitutes a considerable challenge. The carriers confined to nanostructures require a quantum mechanical description in order to properly reflect their wave-like character due to size quantization. The Schrödinger-Poisson system as well as non-equilibrium Green's functions provide a powerful formalism to describe quantum transport in semiconductor structures, however their application to full devices is prohibitively expensive. Since the nanostructures typically constitute only small subregions of the whole device, it is reasonable to use hybrid approaches which combine quantum mechanical descriptions for the confined carriers with (semi-)classical models for the transport of the freely roaming carriers in the barrier material. For the latter one may choose e.g. the van Roosbroeck system [1], which provides a good compromise between accuracy and efficiency and has become the standard model for semi-classical transport simulation. An established approach is the coupling of a transport model with (conventional) rate equations in order to describe the carrier population dynamics within nanostructured domains, e.g. [2], [3]. While this approach works well for QD-layers with high sheet density and quantum wells, the rate equation approach breaks down for systems containing only a single or a few (electronically uncoupled) QDs, since the underlying ensemble averages become invalid in this case [4]. Instead, a master equation approach must be used in order to properly describe the transitions between microstates. We recently employed the coupling of the van Roosbroeck system to a quantum master equation (QME) in order to simulate electrically driven single-photon sources [5]. In this paper, our approach is generalized to a much broader scope of application and put on a more rigorous mathematical basis by the investigation of its fundamental thermodynamic properties.

II. Hybrid quantum-classical model

A. Model equations

We consider a hybrid quantum-classical model that self-consistently couples semi-classical transport theory to a kinetic equation for the quantum mechanical density matrix. The latter one is a Markovian QME that describes the evolution of an open quantum system which interacts with its environment. Our approach is based on the hypothesis that charge carriers can be separated into (free) continuum carriers and (bound) carriers confined to QDs. The model equations read

$$-\nabla\cdot\varepsilon\nabla\phi = q\left(p-n+C+Q\left(\rho\right)\right), \tag{1}$$

$$\partial_t p + \frac{1}{q}\nabla\cdot\mathbf{j}_p = -R - S_p\left(\rho\right), \tag{2}$$

$$\partial_t n - \frac{1}{q}\nabla\cdot\mathbf{j}_n = -R - S_n\left(\rho\right), \tag{3}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = -\frac{i}{\hbar}\left[H,\rho\right] + \mathcal{D}\left(\rho\right). \tag{4}$$

Eqns. (1)–(3) represent the standard van Roosbroeck system, extended by additional terms that constitute the coupling to the QME (4). The system consists of Poisson's eq. (1) for the electric potential ϕ and two continuity eqns. (2)–(3) modeling drift and diffusion of electrons and holes in the

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presence of recombination. The coupling terms are formulated as functionals of the quantum mechanical density matrix ρ. The carrier density $Q(\rho)$ of the quantum system enters Poisson's equation and the carrier capture rates $S_{n/p}(\rho)$ reflect the loss of continuum carriers that are captured to the QDs. We will give general construction rules for the coupling terms respecting the principle of charge conservation.

The state of the quantum system is described by the density matrix ρ which is subject to the QME (4). It describes the evolution of a many-body problem modeling the charges confined to QDs as well as further quasi-particles comprising e.g. cavity photons, phonons or plasmons and exciton-polaritons (dressed states). The Hamiltonian takes the form $H = H_0 + H_I$, where H_0 describes the single-particle energies of the electrons and holes confined to the QDs (and possibly additional species). The interaction Hamiltonian H_I is assumed to commute with the charge number operator $N = n_e - n_h$ such that the Hamiltonian part of the evolution conserves the net charge. This rather weak restriction allows e.g. for Coulomb interaction between the confined carriers (configuration interaction) as well as light-matter interaction.

The non-Hamiltonian part of the evolution generated by Eq. (4) is modeled by a dissipator in Lindblad form [6]

$$\mathcal{D}(\rho) = \sum_{\alpha} \gamma_\alpha \left(A_\alpha \rho A_\alpha^\dagger - \frac{1}{2} \{ A_\alpha^\dagger A_\alpha, \rho \} \right),$$

which is a superoperator acting on the density matrix. The dissipator accounts for dissipative interactions of the quantum system with its environment. The operators A_k are traceless operators on the Hilbert space of the quantum system. Here, $\mathcal{D}(\rho)$ describes in particular carrier capture and escape as well as carrier relaxation processes, spontaneous emission of photons to leaky modes and emission of resonant cavity photons. In the hybrid model (1)–(4) the environment of the quantum system is the spatio-temporally resolved electron-hole plasma which itself is subject to the van Roosbroeck system (1)–(3). The coupling is achieved by formulating the microscopic transition rates $\gamma_\alpha = \gamma_\alpha(n, p, \psi, \nabla\psi)$ as functionals of the free carrier densities and the electric field. The dissipator $\mathcal{D}(\rho)$ is required to satisfy the quantum detailed balance principle with respect to the thermal equilibrium state [7].

B. Thermodynamics

We investigate the system (1)–(4) with respect to its consistency with non-equilibrium thermodynamics. Moreover we give an explicit construction of the equilibrium solution by minimizing the grand canonical potential of the combined quantum-classical system. Finally, explicit conditions for the conservation of the total charge are derived and the entropy production rate of the coupled system is analyzed.

III. Numercial simulation

We apply the model (1)–(4) for the simulation of an electrically pumped single-photon source containing a single QD as optically active element. The hybrid modeling approach allows to compute the essential quantum optical figures of merit

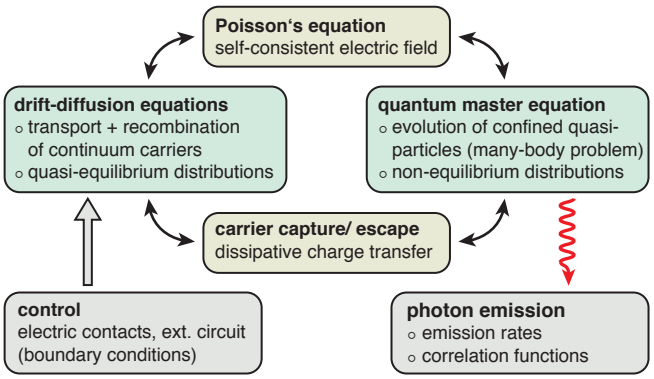

Figure 1. Schematic illustration of the modeling approach: A QME describing a system of quantum dots is self-consistently coupled to the drift-diffusion equations. Both (sub-)systems exchange charge carriers by capture and escape and interact via their self-consistently generated electric field.

such as the single-photon emission rates and the second order intensity correlation function along with a spatially resolved simulation of the current flow. The simulations are carried out using a Voronoï box based finite-volume Scharfetter-Gummel method with implicit Euler time stepping. The numerical results are in good agreement with experimental findings.

IV. Summary

Quantum dot devices can be simulated by a hybrid quantum-classical model, which combines a quantum kinetic many-body problem with semi-classical transport theory. We studied the fundamental thermodynamic properties of the coupled system, in particular the conservation of the total charge and consistency with the second law of thermodynamics. The hybrid model greatly enhances the range of application of semi-classical transport simulations to novel devices such as single-photon sources and QD polariton lasers.

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