Simulation of quantum light sources using the self-consistently coupled Schrödinger-Poisson-Drift-Diffusion-Lindblad system

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***Abstract*—The device-scale simulation of electrically driven quantum light sources based on semiconductor quantum dots requires a combination of the (classical) semiconductor device equations with cavity quantum electrodynamics. In this paper, we extend our previously developed hybrid quantum-classical model system – where we have coupled the drift-diffusion system with a Lindblad-type quantum master equation – by including a self-consistent Schrödinger–Poisson problem. The latter describes the (quasi-)bound states of the quantum dot carriers. The extended model allows to describe the bias-dependency of the emission spectrum due to the quantum confined Stark effect.**

I. Introduction

The currently unfolding "second quantum revolution" aims at the development of novel quantum technologies that exploit inherent quantum mechanical phenomena for communication and information processing tasks. Many applications, such as eavesdropping-secure encryption methods and optical quantum computers, rely on efficient quantum light sources that emit single photons on demand [1]. Semiconductor quantum dots (QDs) have been identified as ideal optically active elements for such devices, as they provide an atom-like discrete energy spectrum and can be directly integrated into semiconductor-based photonic resonators. In the interest of compactness and scalability, electrical carrier injection is highly desirable to overcome the need for external excitation lasers.

On the step from basic research to real world applications, mathematical modeling and numerical simulation can assist the development and optimization of novel device designs. In many well-established simulation tools for optoelectronic devices (e. g., conventional laser diodes, LEDs etc.), the drift-diffusion model is coupled with semi-classical models for the light-matter interaction (e. g., Maxwell–Bloch equations, rate equations) to describe the optically active region. For devices operating in the quantum optical limit, however, the description of the light-matter interaction requires a fully quantum mechanical approach using the framework of cavity quantum electrodynamics [2], which is clearly beyond the standard approach. To meet this requirement, we have developed a hybrid quantum-classical model system [3], that self-consistently couples the drift-diffusion system to a Lindblad-type quantum master equation [4], which describes the microscopic QD-photon system in second quantization. In this paper, we extend our approach by including a self-consistent Schrödinger–Poisson system, to model the energy shifts of the QD carriers in the diode's internal electric field (quantum confined Stark effect).

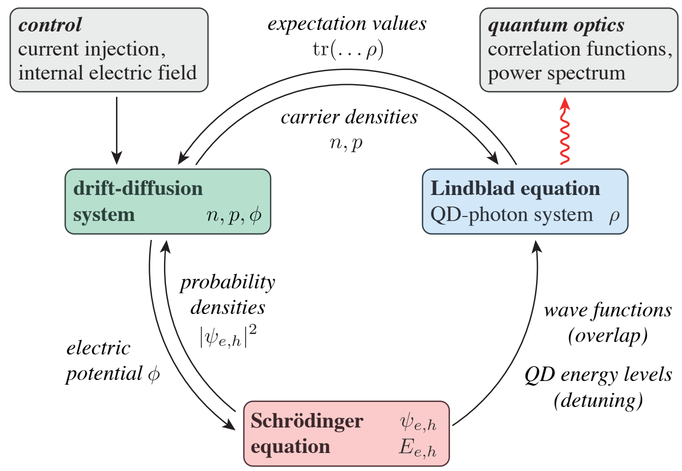

Fig. 1. Schematic illustration of the building blocks and the coupling structure in the Schrödinger-Poisson-Drift-Diffusion-Lindblad system (1)–(5) [5].

II. Model Equations

We describe a comprehensive modeling approach for the simulation of quantum light emitting diodes. The approach is based on the hybrid quantum-classical model system proposed in Ref. [3] and is extended by a self-consistent Schrödinger–Poisson problem modeling the wave functions and energy levels of the (quasi-)bound QD carriers: [5]

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

$$\partial_t n - \frac{1}{q}\nabla\cdot\mathbf{j}_n = -R - S_n, \tag{2}$$

$$\partial_t p + \frac{1}{q}\nabla\cdot\mathbf{j}_p = -R - S_p, \tag{3}$$

$$H_\alpha^0(\phi)\,\psi_\alpha = E_\alpha\psi_\alpha \qquad (\alpha\in\{e,h\}), \tag{4}$$

$$\partial_t\rho = -\frac{i}{\hbar}\,[\mathcal{H},\rho] + \mathcal{D}\rho. \tag{5}$$

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The system comprises the drift-diffusion system (1)–(3) for the transport and recombination dynamics of the continuum electrons and holes, a one-particle Schrödinger equation (4) for each the QD bound electrons and holes, respectively, and a Lindblad-type quantum master equation (5) for the density matrix ρ. A schematic illustration of the "Schrödinger-Poisson-Drift-Diffusion-Lindblad system" (1)–(5) and the interconnection of its building blocks is shown in Fig. 1.

The electrostatic interaction between the freely moving and bound carriers of the system is described by Poisson's Eq. (1), where ϕ is the electric potential, n and p are the densities of (continuum) electrons and holes, C is the doping profile, Q is the charge density of the QD carriers, q is the elementary charge and ε is the material's dielectric constant. The current densities $\mathbf{j}_{n/p}$ in Eqs. (2)–(3) are given by the usual drift-diffusion expressions and R models the (net-)recombination of the continuum carriers. The quantization energy levels and (envelope) wave functions of the QD carriers are determined by the stationary Schrödinger Eq. (4), where the Hamiltonian

$$H_\alpha^0\left(\phi\right) = -\frac{\hbar^2}{2}\nabla\cdot\frac{1}{m_\alpha^*}\nabla + U_\alpha \pm q\phi, \quad \alpha\in\{e,h\}, \tag{6}$$

involves a position-dependent effective mass m_α^*, the QD confinement potential U_α and the electric potential ϕ given by Eq. (1). The Schrödinger Eqs. (4) are solved with outgoing wave conditions on a subset of the full computation domain. In general, this is a non-Hermitian eigenvalue problem that yields complex energy eigenvalues $E_\alpha \in \mathbb{C}$ (quasi-bound states). The many-body Hamiltonian $\mathcal{H}$ in the quantum master Eq. (5) describes the one-particle energy contributions of the QD carriers, the energy of the quantized radiation field, the quantum-mechanical light matter interaction and the Coulomb interaction between the bound carriers in second quantization:

$$\begin{aligned}\mathcal{H} &= \varepsilon_e e^\dagger e + \varepsilon_h h^\dagger h + \hbar\omega_0 a^\dagger a \\ &\quad + \hbar g\left(e^\dagger h^\dagger a + a^\dagger h e\right) - V_{e,h} e^\dagger h^\dagger h e.\end{aligned} \tag{7}$$

Here, a and $a^\dagger$ are the bosonic annihilation and creation operators of the cavity photons and e (h) and $e^\dagger$ ($h^\dagger$) are the respective fermionic operators for the QD-bound electrons (holes). Moreover, $\hbar\omega_0$ is the resonance energy of the cavity, g is the light-matter coupling constant and $V_{e,h}$ is the QD exciton binding energy. The one-particle energies $\varepsilon_\alpha = \mathrm{Re}\left(E_\alpha\right)$ are taken as the real values of the complex eigenvalues determined by Eq. (4). The dissipation superoperator $\mathcal{D}\left(\rho\right)$ in Eq. (5) models the irreversible coupling of the quantum system to its macroscopic environment. This include the scattering of carriers from the continuum to the QD states, spontaneous decay of the QD exciton (to waste modes), emission of cavity photons and pure dephasing. The respective transition rates are driven by the classical carrier densities n, p in the vicinity of the QD and involve the corresponding overlap integrals using the wave functions from Eq. (4). Finally, the feedback of the quantum system on its macroscopic environment is mediated by the charge density Q and the scattering rates $S_{n,p}$. The corresponding expressions are constructed following Refs. [3, 5] as expectation values of the respective operators.

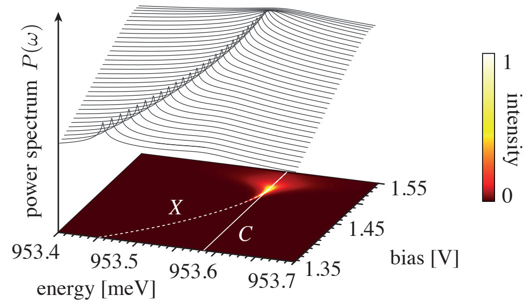

Fig. 2. Calculated power spectrum $P\left(\omega\right)$ as a function of the applied bias. The QD exciton (X) is tuned into resonance with a (broad) photonic cavity resonance (C). The single-photon generation rate reaches a maximum at about 1.5 V and then decreases due to excitation-induced dephasing at high currents.

III. Results

We demonstrate our approach by numerical simulations of a single-photon emitting diode. As indicated in Fig. 1, the model system (1)–(5) allows to evaluate the quantum optical features of the system in dependence on the state of its macroscopic environment. In particular, we compute the power spectrum

$$P\left(\omega\right) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\tau\, e^{-i\omega\tau}\left\langle a^\dagger\left(\tau\right)a\left(0\right)\right\rangle \tag{8}$$

(Fourier transform of the first-order autocorrelation function of the cavity photons) as a function of the applied bias. The result is shown in Fig. 2, where the QD exciton is tuned into resonance with the photonic resonator mode via the quantum confined Stark effect. Moreover, thanks to the fully self-consistent coupling of the quantum mechanical subsystem and its macroscopic environment (via Q and $S_{n/p}$), our simulations reveal a noticeable impact of the QD on the current paths.

IV. Outlook and conclusions

We have extended the hybrid quantum-classical model system for the simulation of quantum light sources introduced in Ref. [3] by a self-consistent Schrödinger–Poisson problem. The extension allows to describe important phenomena such as the quantum confined Stark effect and might be used to study spectral diffusion of the emission energy in a future work.

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