Modeling and simulation of injection dynamics for quantum dot based single-photon sources

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***Abstract*—Single semiconductor quantum dots embedded in p-i-n diodes have been demonstrated to operate as electrically driven single-photon sources. By means of numerical simulations one can explore the limitations in the carrier injection dynamics and further improve the device technology. We propose a comprehensive modeling approach coupling the macroscopic transport of bulk carriers with an open quantum system to describe the essential physics of such devices on multiple scales.**

I. Introduction

Single-photon sources (SPSs) are key components for many interesting applications in the field of quantum cryptography, optical quantum computing and quantum metrology [1]. Self-assembled semiconductor quantum dots (QDs) are excellent candidates for the realization of SPSs since they show a (tailorable) discrete energy spectrum, narrow linewidth and can be directly fabricated within semiconductor microcavities using well established growth techniques. In the recent years several authors have shown that electroluminescence from single QDs within the intrinsic region of a p-i-n diode acts as an electrically driven SPS (e.g. [2]–[5]) with single-photon emission rates ranging from several MHz up to a few GHz. For realistic applications high single-photon emission rates along with a high single-photon purity and indistinguishability are desirable, while simultaneously a deterministic growth technology suitable for electrical injection is required.

Modeling and numerical simulation of electronic transport in SPSs can help to theoretically explore the limits and bottlenecks in the carrier injection dynamics in terms of high repetition frequency and emission time jitter reduction for various device concepts. Here we aim for a comprehensive modeling approach describing the spatial bulk carrier transport and the carrier-scattering cascade over 2D wetting layer (WL) states into the QD. The carrier recombination kinetics of the excitonic states in the QD will be described by a quantum mechanical density matrix. A schematic representation of our approach is depicted in Fig. 1.

II. Model

In a semi-classical framework, the transport and recombination dynamics of bulk carriers in a self-consistent electric field is typically described by the van Roosbroeck system [6]. In order to model the combined bulk-WL-QD system

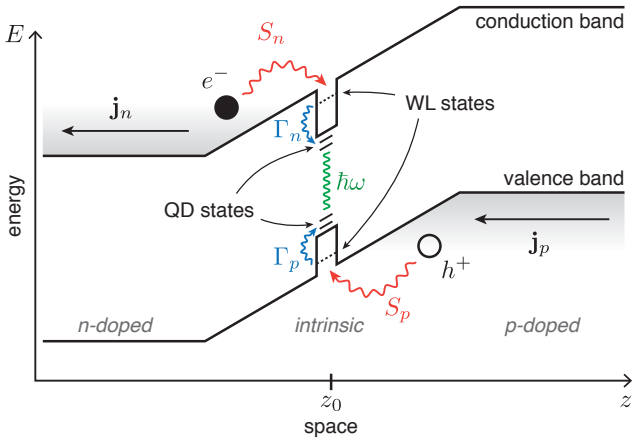

Figure 1. Schematic representation of the bulk transport model coupled to a WL and a single QD in the intrinsic domain of a GaAs-based p-i-n diode. The interaction of bulk carriers and carriers in the bound states of the nanostructures is mediated by the capture and escape rates $S_{n/p}$ and $\Gamma_{n/p}$.

one has to extend the standard drift-diffusion transport model by additional terms and equations describing the occupation dynamics of the nanostructures stimulated by cascaded carrier capture and escape events (as e.g. in [7]). We propose a multi-species model separating the carriers in the bulk, WL and QD states and couple them by phenomenological scattering terms. The electric potential ψ obeys Poisson's equation

$$-\nabla\cdot\varepsilon\nabla\psi = q\left(p-n+N_D^+-N_A^-\right)+ \\ +q\delta\left(z-z_0\right)\left(p_{\mathrm{WL}}-n_{\mathrm{WL}}\right)+q\delta\left(\mathbf{r}-\mathbf{r}_0\right)Q\left[\rho\right] \tag{1}$$

where the electric field is generated by the net charge density given by the density of bulk carriers p, n, the WL carrier densities $p_{\mathrm{WL}}, n_{\mathrm{WL}}$ and the net density of charged complexes within the QD given by $Q[\rho]$. Here the WL is regarded as a charged interface and the QD is assumed to be 0-dimensional point source. The transport of the bulk carriers is described by a continuity equation for each carrier species

$$q\partial_t p+\nabla\cdot\mathbf{j}_p = -qR-q\delta\left(z-z_0\right)S_p \tag{2a}$$
$$q\partial_t n-\nabla\cdot\mathbf{j}_n = -qR-q\delta\left(z-z_0\right)S_n \tag{2b}$$

where the current densities are modeled in a standard way as drift-diffusion currents obeying a generalized Einstein relation.

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The net recombination rate of the bulk carriers is described by R and $S_{n/p}$ models the carrier capture and escape processes into and out of the WL according to [8]. These scattering rates couple the transport equations of the bulk carriers with rate equations for the carriers in the WL states

$$q\partial_t p_{\mathrm{WL}} + \nabla_{\parallel} \cdot \mathbf{j}_p^{\mathrm{WL}} = -qR_{\mathrm{WL}} + qS_p - q\delta\left(\mathbf{r}-\mathbf{r}_0\right)\Gamma_p \quad (3a)$$

$$q\partial_t n_{\mathrm{WL}} - \nabla_{\parallel} \cdot \mathbf{j}_n^{\mathrm{WL}} = -qR_{\mathrm{WL}} + qS_n - q\delta\left(\mathbf{r}-\mathbf{r}_0\right)\Gamma_n \quad (3b)$$

where the transport is considered only in a plane parallel to the growth direction. As above, R_{WL} models the net recombination rate of the WL carriers and $\Gamma_{n/p}$ mediates the relaxation into and out of the QD states.

In order to describe the various, interacting multi-particle configurations of the QD, a modeling approach based on a density matrix formalism has been proven useful. We regard the QD as an open quantum system and describe its time evolution by the quantum master equation

$$\dot{\rho} = -\frac{i}{\hbar}\left[H,\rho\right] + \mathcal{D}\rho \quad (4)$$

where ρ is the quantum mechanical density matrix, H denotes the systems Hamiltonian and the dissipator term

$$\mathcal{D}\rho = \sum_{\nu} \gamma_\nu\left(p_{\mathrm{WL}}, n_{\mathrm{WL}}, \psi\right)\mathcal{L}\left[a_\nu\right]\rho$$

models various dissipative interactions of the QD with its environment. Here $\mathcal{L}$ denotes the Lindblad superoperator [9]. In the low Q resonator regime it is sufficient to merely describe the electronic configuration of the QD by the Hamiltonian. The light-matter interaction, the carrier injection as well as non-radiative decay processes can be regarded as weak interactions of the QD with its environment. Therefore their description is carried out by means of dissipator terms with appropriate models for the respective rates γ_ν. The single-particle states of the QD are modeled by a confinement potential as in [10] and the Coulomb interaction is treated in an approximative way using the approach presented in [11]. Taking only the multi-particle ground-states up to 4 particles into account (including dark and bright excitons, trions and the biexciton), we come up with a (comparatively) simple system describing the QD occupation probability and the recombination kinetics. A diagram of the QD configurations is illustrated in Fig. 2. Within the density matrix formalism the computation of the second order correlation function of any emission line can be carried out by the quantum regression theorem. [9]

A particularity of InGaAs-QD based SPSs is the extremely low operation temperature, which is typically in the range of 5-30 K [4] to ensure narrow linewidths by suppressing acoustic phonons. The computations in this cryogenic limit are very challenging for the numerical algorithms for various reasons [12], [13]. The simulations are performed by using a Voronoï box based finite volumes scheme with a modified Scharfetter-Gummel method for Fermi-Dirac statistics.

III. Summary

The simulation of electrically driven QD-based single-photon emitters requires the coupling of the drift-diffusion transport model to a quantum mechanical model of the QD. Quantum master equations of Lindblad type provide a simple and effective approach to simulate the interaction of multiple QD configurations with its dynamic environment.

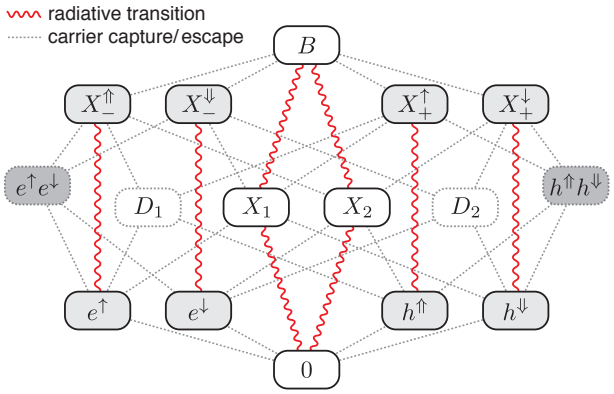

Figure 2. Diagram of the multi-particle configurations of the QD considered in the model. The occupation probabilities of the states are described by the density matrix ρ obeying the quantum master equation (4). The radiative transitions and the excitation scheme (carrier capture and escape processes) are indicated as wavy and dashed lines, respectively.

Acknowledgment

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