

Weierstrass Institute for **Applied Analysis and Stochastics** 

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Modeling and simulation of electrically driven quantum light sources From classical device physics to open quantum systems

Semiconductor Nanophotonics SFB 787 Leibniz Association

### Motivation

Semiconductor quantum optics is on the leap from the lab to real world applications. In order to advance the **development of novel devices** such as quantum light sources and nanolasers based on semiconductor quantum dots embedded in dielectric micro-cavities, device engineers will need simulation tools that combine classical device physics with cavity quantum electrodynamics. We connect the fields of semi-classical semiconductor transport theory and the theory of open quantum systems to meet this requirement.



### Current spreading in an oxide-confined pn-diode

• site-controlled QD nucleation above oxide aperture via buried stressor



optical activity of parasitic QDs Ο rapid lateral curent spreading above Ο oxide (no bulk recombination)



## Hybrid quantum-classical modeling approach

Comprehensive multi-scale simulation approach for QD-based devices for quantum optics: Self-consistent coupling of **drift-diffusion system** (semi-classical charge carrier transport) with **Lindblad master equation** for dissipative QD-photon system: Spatially resolved current flow in realistic semiconductor device geometries and quantum optics out of one box!

Hybrid quantum classical model  $-\nabla \cdot \varepsilon \nabla \phi = q \left( C + p - n + Q(\rho) \right)$  $\partial_t n - \frac{1}{q} \nabla \cdot \mathbf{j}_n = -R - S_n(\rho; n, p, \phi)$  $\partial_t p + \frac{1}{q} \nabla \cdot \mathbf{j}_p = -R - S_p(\rho; n, p, \phi)$  $\partial_t \rho = -\frac{i}{\hbar} [H, \rho] + \mathcal{D}(n, p, \phi) \rho$ 



• modified doping profile  $\Rightarrow$  electrical pumping of single QDs



Strittmatter et al., *Appl. Phys. Lett.* **100**, 093111 (2012) Unrau et al., *Appl. Phys. Lett.* **101**, 211119 (2012) Kantner et al., *IEEE Trans. Electron Dev.* **63**, 2036 (2016)

# **Consistency with (non-)equilibrium thermodynamics**

Consistency with fundamental laws of (non-)equilibrium thermodynamics is considered as a guiding principle for the formulation of the quantum-classical system. By construction, the system satisfies the **conservation of charge** and thermodynamic principles such as **microscopic reversibility** in the thermodynamic equilibrium and the second law of thermodynamics.

minimize (hybrid) grand potential in 0 thermodynamic equilibrium

$$\Phi = \mathcal{F}(n, p, \rho) - \mu_{eq} \int_{\Omega} d^3 r \left( n - p - Q(\rho) \right)$$

(quantum) detailed balance relation

 $\mathcal{D}(n_{\mathrm{eq}}, p_{\mathrm{eq}}, \phi_{\mathrm{eq}})\rho_{\mathrm{eq}} = 0$ 

#### entropy production rate

$$\dot{\mathcal{S}}_{\text{tot}} = \frac{1}{T} \int_{\Omega} d^3 r \, (\mu_c - \mu_v) \, R + \frac{1}{qT} \int_{\Omega} d^3 r \, (\mathbf{j}_n \cdot \nabla \mu_c + \mathbf{j}_p \cdot \nabla \mu_v) \\ + k_B \, \text{tr} \left( \left[ \log \rho - \beta H \right] \mathcal{D}_0 \rho \right) \\ + k_B \, \text{tr} \left( \left[ \log \rho - \log \rho_e^*(n, p, \phi) \right] \mathcal{D}_e(n, p, \phi) \rho \right) \\ + k_B \, \text{tr} \left( \left[ \log \rho - \log \rho_h^*(n, p, \phi) \right] \mathcal{D}_h(n, p, \phi) \rho \right)$$

 $\partial_t z = (\mathbb{J}(z) - \mathbb{K}(z)) D\mathcal{F}(z)$ • gradient structure

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## Simulation results







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