Weierstraß-Institut
für Angewandte Analysis und Stochastik
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Towards doping optimization of semiconductor lasers

Dirk Peschka, Nella Rotundo, Marita Thomas

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Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
email: dirk.peschka@wias-berlin.de
email: nella.rotundo@wias-berlin.de
email: marita.thomas@wias-berlin.de

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Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 20372-303
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

We discuss analytical and numerical methods for the optimization of optoelectronic devices by performing optimal control of the PDE governing the carrier transport with respect to the doping profile. First, we provide a cost functional that is a sum of a regularization and a contribution, which is motivated by the *modal net gain* that appears in optoelectronic models of bulk or quantum-well lasers. Then, we state a numerical discretization, for which we study optimized solutions for different regularizations and for vanishing weights.

1 Introduction

Studies of semiconductor device optimization via optimal control methods have been the subject of a number of previous studies, cf. e.g. [6, 7, 8]. In recent years there has been an increase in research on optoelectronic devices, e.g. aimed at on-chip integration of lasers in order to increase communication bandwidths for computing or telecommunication applications. For example, it has been demonstrated recently that germanium can be used as an optically active medium, however, advanced engineering techniques such as high doping or application of large strain, are necessary to improve optical properties of laser cavities [1].

In the following, we present our first steps towards the optimal control of an optoelectronic device. In Sec. 2 we introduce a model that has been used to describe optical modes, charge transport and spontaneous emission in the cross-section of an edge-emitting laser. We first simplify this model to the extend we believe is reasonable for a laser below lasing threshold. For this model we discuss well-posedness in Sec. 3 relying on well-known existence results cf. e.g. [4, 12, 16, 17]. In Sec. 4 we set up an optimal control problem with the goal to improve the optical properties of the laser. Finally, in Sec. 5 we discuss the feasibility of the optimization concept at the hand of 1D-examples.

2 Mathematical model

The state of a semiconductor in a bounded domain $\Omega \subset \mathbb{R}^d$, with $d = 1, 2, 3$ is described by the electrostatic potential ψ and by the carrier densities n, p for the electrons in the conduction band and holes in the valence band, respectively. Steady-state solutions (ψ, n, p) solve the van Roosbroeck system [4], which after non-dimensionalization using $[x] = l$, $[\psi] = U_T$, $[n, p, C] = N_0$ reads

$$-\Delta\psi = q(C + p - n), \qquad \nabla \cdot j_n = R, \qquad \nabla \cdot j_p = -R. \tag{1a}$$

The current densities for electrons $j_n = -\mu_n n \nabla \varphi_n$ and holes $j_p = -\mu_p p \nabla \varphi_p$ are proportional to the gradients of the quasi-Fermi potentials φ_n and φ_p, which are related to the carrier densities through the equation of state

$$n = n_i \exp(\psi - \varphi_n), \qquad \text{and} \qquad p = n_i \exp(\varphi_p - \psi). \tag{1b}$$

With C we denote the given doping concentration. In this model we rescaled the dimensional mobilities by μ_0, recombination rates by $R_0 = U_T \mu_0 N_0 / l^2$, intrinsic densities by N_0, and defined $q = l^2 q_e N_0 / (U_T \varepsilon)$ and $U_T = k_B T / q_e$. At Ohmic contacts Γ_D these equations are supplemented with the following special type of Dirichlet boundary conditions

$$\psi = \psi_{\mathrm{bi}} + \psi_{\mathrm{ext}}, \quad \varphi_n = \psi_{\mathrm{ext}}, \quad \varphi_p = \psi_{\mathrm{ext}}, \quad \text{on } \Gamma_{\mathrm{D}}, \tag{1c}$$

using the built-in voltage ψ_{bi} and the given external voltage ψ_{ext}, and on the insulating part with

$$\nabla \psi \cdot \nu = j_n \cdot \nu = j_p \cdot \nu = 0, \quad \text{on } \Gamma_{\mathrm{N}}. \tag{1d}$$

Rewriting the fluxes in (1) in terms of the densities n, p, one arrives at the well-known form

$$j_n = -\mu_n (n \nabla \psi - \nabla n), \qquad\qquad j_p = -\mu_p (p \nabla \psi + \nabla p), \tag{2}$$

and at Ohmic contacts the boundary conditions become

$$\psi = \psi_{\mathrm{bi}} + \psi_{\mathrm{ext}} =: \psi_{\mathrm{D}}, \quad n = n_i e^{\psi_{\mathrm{bi}}} =: n_{\mathrm{D}}, \quad p = n_i e^{-\psi_{\mathrm{bi}}} =: p_{\mathrm{D}}, \quad \text{on } \Gamma_{\mathrm{D}}, \tag{3}$$

so that we have $np = n_i^2$ at Γ_D.

In addition to the electronic transport model (1), an optoelectronic model needs to take into account radiative recombination processes and should, in particular, capture the number of coherent photons S generated by stimulated emission. Analogously to [9] we introduce the optical modes Ψ as solutions of a Helmholtz eigenvalue problem, which prototypically for TE modes reads

$$\left[\nabla^2 + \left(n_r + \tfrac{i}{2}(g - \ell - \ell_1)\right)^2\right] \Psi = \beta^2 \Psi,$$

with n_r the refractive index of the material. The imaginary part of the eigenvalue enters the stationary balance of stimulated emission and spontaneous emission r_{sp} as $0 = (2\mathrm{Im}\beta - \ell_2)S + r_{\mathrm{sp}}$, where ℓ_1, ℓ_2 constitute additional loss mechanisms not consider here. With g and ℓ we denote the *gain* and, as a representative loss mechanism, the *free carrier absorption*, which encodes the rate at which photons S are created and annihilated and which both depend on carrier densities, i.e. $g = g(n, p)$ and $\ell = \ell(n, p)$. Motivated by one of our previous studies [2] we use

$$g(n,p) := g_0 (np)^{\delta} - g_1 (np)^{\delta - 1}, \tag{4a}$$
$$\ell(n,p) := f_n n + f_p p, \tag{4b}$$

where $g_0, g_1, f_n, f_p > 0, \delta \in (0, 1/2)$ are material dependent parameters (possibly depending on wavelength, material quality, temperature, mechanical strain etc.) and which in the following are taken to be constant in space. By a perturbation argument one can show that the imaginary part of the eigenvalue can be approximated

$$\mathrm{Im}\beta \simeq \int_{\Omega} (g(n,p) - \ell(n,p))|\Psi|^2 \,\mathrm{d}x, \tag{5}$$

where, to leading order, the form of Ψ does not depend on the charge distribution.

The recombination-generation term $R = R_{\mathrm{norad}} + R_{\mathrm{rad}}$ in (1) takes into account different non-radiative and radiative recombination processes. The non-radiative Auger and Shockley-Read-Hall recombination terms are of the form $R_{\mathrm{norad}} = \tilde{R}(n,p)(np - n_i^2)$. In addition we have radiative recombinations $R_{\mathrm{rad}} = \tilde{R}_{\mathrm{spont}}(np - n_i^2) + R_{\mathrm{stim}}(n,p)$. In addition to spontaneous recombination it contains the main ingredient for a laser, the stimulated radiative recombination

$$R_{\mathsf{stim}}(n,p) \simeq g(n,p)|\Psi|^2 S, \tag{6}$$

which has the stimulated emission term $\mathrm{Im}\beta$ in the algebraic equation for S as a counterpart. For the purpose of this paper we consider the optimization of a laser below threshold $0 < S \ll 1$. From a practical point of view this implies that we neglect the influence of the optics on the electronic transport and set $S = 0$, whereas it is taken into account in the optimization by using $\mathrm{Im}\beta$ in (5) as one part of the cost functional. Such a strategy is aimed at lowering the threshold current of a semiconductor laser.

3 The existence of solutions

In the subsequent sections we assume that

- the domain Ω is bounded in $\mathbb{R}^d$, $d \in \{1,2,3\}$, with Lipschitz boundary such that $\Gamma_{\mathrm{D}} \neq \emptyset$ and $\Gamma_{\mathrm{N}} = \partial\Omega \backslash \Gamma_{\mathrm{D}}$, (7)
- $R(n,p) = \tilde{R}(n,p)(np - n_i^2)$ with $\tilde{R} : [0,\infty)^2 \to [0,\infty)$ continuously.

In order to account for general Dirichlet data $(\psi_{\mathrm{D}}, n_{\mathrm{D}}, p_{\mathrm{D}})$, we shall understand from now on $\xi_{\mathrm{D}} = (\psi_{\mathrm{D}}, n_{\mathrm{D}}, p_{\mathrm{D}})$ as the extension of the data prescribed on Γ_{D} into the domain Ω. The special case of Ohmic contacts (1c) is included the existence Theorem 1. Moreover, we introduce $H^1_{\mathrm{D}}(\Omega) := \{u \in H^1(\Omega),\, u = 0 \text{ on } \Gamma_{\mathrm{D}}\}$. Then we set

$$\mathbf{H} := [H^1(\Omega)]^3, \quad \mathbf{X} := [H^1_{\mathrm{D}}(\Omega) \cap L^\infty(\Omega)]^3, \quad \mathbf{C} \in \{H^1(\Omega), L^p(\Omega) \text{ s.t. } p > d/2\}\,. \tag{8}$$

Note that we want to keep the space $\mathbf{C}$ as general as possible in order to allow for some freedom in the choice of the cost functional later on in Sections 4 & 5. In order to specify our notion of solution we shall interprete the system (1a,2,3) as an operator

$$\rho_{\mathrm{vR}}(\xi_{\mathrm{D}};\cdot,\cdot) : \mathbf{X}\times\mathbf{C} \to [H^1(\Omega)^*]^3,\ \rho_{\mathrm{vR}}(\xi_{\mathrm{D}};\xi,C) := \begin{pmatrix} -\Delta(\psi+\psi_{\mathrm{D}}) - q(C+p+p_{\mathrm{D}}-n-n_{\mathrm{D}}) \\ \nabla\cdot j_n - R \\ \nabla\cdot j_p + R \end{pmatrix},$$

$$\text{where } j_n := \nabla(n+n_{\mathrm{D}}) + (n+n_{\mathrm{D}})\nabla(\psi+\psi_{\mathrm{D}})\,,\ j_p := -\nabla(p+p_{\mathrm{D}}) + (p+p_{\mathrm{D}})\nabla(\psi+\psi_{\mathrm{D}}) \tag{9}$$

with $\xi = (\psi, n, p) \in \mathbf{X}$ and $H^1(\Omega)^*$ the dual of $H^1(\Omega)$. In this way, a suitable notion for solutions of the boundary value problem (1) can be stated as follows.

Definition 1 (Solution for the boundary value problem (1))**.** *For the given data* $C \in \mathbf{C}$ *and* $\xi_\mathrm{D} = (\psi_\mathrm{D}, n_\mathrm{D}, p_\mathrm{D}) \in [H^1(\Omega) \cap L^\infty(\Omega)]^3$ *a triple* $\xi = (\psi, n, p) \in \mathbf{X}$ *is a solution to the boundary value problem of the van Roosbroeck system* (1) *if*

$$\rho_\mathrm{vR}(\xi_\mathrm{D}; \psi, n, p, C) = \mathbf{0} \quad \textit{in } [H^1(\Omega)^*]^3 \,. \tag{10}$$

Arguing along the lines of [4, 17, 12, 7] the following existence result can be obtained.

Theorem 1 (Existence of solutions)**.** *Let* (7) *be satisfied and* $\rho_\mathrm{vR}(\xi_\mathrm{D}, \cdot, \cdot) : \mathbf{X} \times \mathbf{C} \to [H^1(\Omega)^*]^3$ *as in* (8) & (9)*. Then for all given data* $C \in \mathbf{C}$ *and* $(\psi_\mathrm{D}, n_\mathrm{D}, p_\mathrm{D}) \in [H^1(\Omega) \cap L^\infty(\Omega)]^3$ *such that*

$$\|\psi_\mathrm{D}\|_{L^\infty(\Omega)} \le K, \quad \textit{and} \quad \tfrac{1}{K} \le n_\mathrm{D}, p_\mathrm{D} \le K \quad \textit{a.e. in } \Omega \tag{11}$$

for some $K \ge 1$*, there exists a triple* $(\psi, n, p) \in \mathbf{X}$ *such that* (10) *is satisfied and*

$$\|(\psi, n, p)\|_\mathbf{X} \le L \quad \textit{as well as} \quad \tfrac{1}{L} \le n, p \le L \quad \textit{a.e. in } \Omega \tag{12}$$

with a constant $L = L(\Omega, K, \|C\|_\mathbf{C}) \ge 1$*.*

For the shortness of the presentation we shall not give a full proof of the existence Theorem 1, but just outline the main ideas in Remark 2 and rather refer the reader to [4, Sec. 3.2] or [17, 12] for further details. However, it is important to note that the bounds on the given data (11) and the choice of $\mathbf{C}$ according to (8) allow us to find the bounds (12) on the solutions (ψ, n, p). This information will play an important role in the optimization lateron. More precisely, introducing, in accordance with the bounds (12), the topology τ_vR

$$(\psi_k, n_k, p_k, C_k) \overset{\tau_\mathrm{vR}}{\to} (\psi, n, p, C) \;\Leftrightarrow\; \begin{cases} (\psi_k, n_k, p_k) \rightharpoonup (\psi, n, p) & \text{in } [H^1(\Omega)]^3, \\ (\psi_k, n_k, p_k) \overset{*}{\rightharpoonup} (\psi, n, p) & \text{in } [L^\infty(\Omega)]^3, \\ (\psi_k, n_k, p_k) \to (\psi, n, p) & \text{in } [L^q(\Omega)]^3 \text{ for all } q \in (1, \infty), \\ \qquad C_k \rightharpoonup C & \text{in } \mathbf{C} \end{cases} \tag{13}$$

and the set

$$\mathbf{S}_\mathrm{vR} := \{(\xi, C) \in \mathbf{X} \times \mathbf{C},\; (\xi, C) \text{ satisfy (10) \& (12) with } \xi_\mathrm{D} \text{ as in (11)}\}\,, \tag{14}$$

it can be shown, thanks to (12), that $\mathbf{S}_\mathrm{vR}$ is compact in $\mathbf{H} \times \mathbf{C}$ with respect to the topology τ_vR. This will be the crucial ingredient to verify the existence of a solution for the optimization problem treated in Sec. 4.

Proposition 1 (Compactness of $\mathbf{S}_\mathrm{vR}$)**.** *The set* $\mathbf{S}_\mathrm{vR}$ *defined in* (14) *is compact in* $\mathbf{H} \times \mathbf{C}$ *with respect to the topology* τ_vR*.*

Proof: Consider a sequence $(\hat\psi_k, \hat n_k, \hat p_k, \hat C_k)_k \subset \mathbf{S}_\mathrm{vR}$ such that $\|(\hat\psi_k, \hat n_k, \hat p_k, \hat C_k)\|_{\mathbf{H}\times\mathbf{C}} \le M$ for a constant $M < \infty$. Thus, $\|\hat C_k\|_\mathbf{C} \le M$ and hence, by (12), also $\|(\hat\psi_k, \hat n_k, \hat p_k)\|_{[L^\infty(\Omega)]^3} \le L(M)$ and $1/L(M) \le \hat n_k, \hat p_k \le L(M)$ a.e. in Ω. By the reflexivity of $[H^1(\Omega)]^3$ we find a (not relabelled) subsequence $(\hat\psi_k, \hat n_k, \hat p_k)_k$ and a triple $(\hat\psi, \hat n, \hat p) \in [H^1(\Omega)]^3$ such that

$(\hat{\psi}_k, \hat{n}_k, \hat{p}_k) \rightharpoonup (\hat{\psi}, \hat{n}, \hat{p})$ in $[H^1(\Omega)]^3$. By the compact embedding $[H^1(\Omega)]^3 \Subset [L^2(\Omega)]^3$ we have that $(\hat{\psi}_k, \hat{n}_k, \hat{p}_k) \to (\hat{\psi}, \hat{n}, \hat{p})$ in $[L^2(\Omega)]^3$, which can be upgraded to strong convergence in $[L^q(\Omega)]^3$ for any $q \in (1, \infty)$ thanks to the uniform L^∞-bound. Indeed, this bound also implies the weak-star convergence in $L^\infty(\Omega)$ of a further subsequence. Upon extrating a further subsequence that converges pointwise a.e. in Ω we deduce that $1/L(M) \leq \hat{n}, \hat{p} \leq L(M)$ a.e. in Ω. Finally, using Banach-Alaoglu's theorem, the uniform bound of $(\hat{C}_k)_k$ in $\mathbf{C}$, as a dual of a separable Banach space, allows us to conclude the convergence of a subsequence to a limit $\hat{C} \in \mathbf{C}$. In conclusion, we have obtained that also the limit $(\hat{\psi}, \hat{n}, \hat{p}, \hat{C})$ satisfies (12).

It remains to show that the limit $(\hat{\psi}, \hat{n}, \hat{p}, \hat{C})$ complies with (10). Thanks to the first and the fourth convergence property of (13) we find that $\hat{\psi}$ is a weak solution of the Poisson equation in (1), i.e. the first line of system (10), with right-hand side $q(\hat{C} - \hat{n} - n_{\mathrm{D}} + \hat{p} + p_{\mathrm{D}})$. In order to show that $(\hat{\psi}, \hat{n}, \hat{p})$ also solve the corresponding continuity equations note that with $(\hat{n}_k, \hat{p}_k)_k$ satisfying (12) we have $|R| \leq \max_{(n,p) \in [1/L, L]} \tilde{R}(n + n_{\mathrm{D}}, p + p_{\mathrm{D}}) \left((L+K)^2 - n_i^2\right)$ pointwise a.e. in Ω, uniformly for all $k \in \mathbb{N}$. Owing to the strong L^q-convergence ensured in the third line of (13), we may extract a not relabelled subsequence such that $(\hat{n}_k, \hat{p}_k) \to (\hat{n}, \hat{p})$ pointwise a.e. and since all the reaction terms are continuous according to (7), we find that $R(\hat{n}_k + n_{\mathrm{D}}, \hat{p}_k + p_{\mathrm{D}}) \to R(\hat{n} + n_{\mathrm{D}}, \hat{p} + p_{\mathrm{D}})$ along this subsequence. Thus, thanks to the pointwise uniform bound, we find with the aid of the dominated convergence theorem that $\int_\Omega R(\hat{n}_k + n_{\mathrm{D}}, \hat{p}_k + p_{\mathrm{D}}) v \, \mathrm{d}x \to \int_\Omega R(\hat{n} + n_{\mathrm{D}}, \hat{p} + p_{\mathrm{D}}) v \, \mathrm{d}x$ for any test function $v \in H^1(\Omega)$, hence the convergence of the right-hand sides in the second and third line of (10). Finally, we obtain the convergence of the corresponding left-hand sides by weak-strong convergence arguments using the first of (13) and that $\|(\hat{n}_k - \hat{n}) v\|^2_{L^2(\Omega)} \leq \|v\|^2_{L^{2^*}(\Omega)} \|\hat{n}_k - \hat{n}\|^2_{L^{(2^*)'}(\Omega)} \to 0$ thanks to the third of (13), and the corresponding argument for the hole density. Thus, $(\hat{\psi}, \hat{n}, \hat{p}, \hat{C})$ satisfies (10) and alltogether we have verified that $(\hat{\psi}, \hat{n}, \hat{p}, \hat{C}) \in \mathbf{S}_{\mathrm{vR}}$. ∎

Remark 1 (Comments on the uniqueness of solutions to (10) and its effect on optimization)**.** *Uniqueness of the solution has been proved in [12] under additional smallness assumptions on the Dirichlet data and restrictions on K in* (11) *which ensure that the applied voltage is sufficiently small and hence keep the carrier densities solving* (10) *sufficiently close to the thermal equilibrium state. Further away from equilibrium, uniquess is in general not to be expected. This has the effect that also an optimization problem based on* (10) *may admit multiple solutions. Also observe that, due to the quasilinear character of the current continuity equations, it is unclear whether $\mathbf{S}_{\mathrm{vR}}$ from* (14) *forms a convex set. This spoils the uniqueness of a minimizer, or at least its verification, for an optimization problem involving functionals with equality constraint* (10)*, even if the functional itself is strictly convex. We refer to [8, Sec. 2], where the non-uniqueness of a minimizer has been demonstrated for a particular choice of the cost functional.*

In order to convince the reader that the bounds (12) indeed hold true for the given data chosen in accordance with (11) and $\mathbf{C}$ as in (8), we shall here outline the main steps of the existence proof leading to (12).

Remark 2 (Comments on the existence proof)**.** *We refer to [4, Sec. 3] for all the details of the existence proof, which may in fact be carried out using the so-called Slotboom variables $\tilde{\psi}, u, v$ such that $\tilde{\psi} = \psi + \psi_{\mathrm{D}}$, $n + n_{\mathrm{D}} = n_i \exp(\tilde{\psi}) u$ and $p + p_{\mathrm{D}} = n_i \exp(-\tilde{\psi}) v$. The bounds* (11) *on the Dirichlet data $n_{\mathrm{D}}, p_{\mathrm{D}}$ in fact ensue from analogous bounds for the Dirichlet data*

$u_{\mathrm{D}}, v_{\mathrm{D}}$ for u, v. The main idea is to apply a fixed point argument based on Schauder's fixed point theorem using a decoupled iteration scheme. More precisely, at iteration step $j \in \mathbb{N}$, one keeps the variables $u_{j-1}, v_{j-1} \in H^1(\Omega) \cap L^\infty(\Omega)$ (satisfying bounds analogous to (12) *with constants C_1, C_2, C_3) fixed in the Poisson equation, i.e. one seeks a solution to the problem $\Delta\tilde{\psi} = q(n_i \exp(\tilde{\psi})u_{j-1} - n_i \exp(-\tilde{\psi})v_{j-1} - C)$, (+ corresponding boundary conditions). For this modified PDE the existence of a unique solution $H_1(u_{j-1}, v_{j-1}) = \tilde{\psi}_j \in H^1(\Omega)$ can be proved using monotone operator theory. Thanks to the Stampacchia method [13] it is possible upgrade this solution $\tilde{\psi}_j$ to be bounded in $L^\infty(\Omega)$ by a constant which continuously depends on the $L^p(\Omega)$-norm (hence $\mathbf{C}$-norm) of the doping function, on the bound corresponding to K for the Dirichlet datum, and on the space dimension, cf. also [11, 12]. Subsequently one may use $\tilde{\psi}_j$ as an input for the equations for the (u, v)-variables (corresponding to the carrier transport equations), hereby suitably linearizing the recombination rate. In this way, one seeks a solution (u_j, v_j) for the system $\operatorname{div} \mu_n \exp(\tilde{\psi}_j)\nabla u = \tilde{R}(\tilde{\psi}_j, u_{j-1}, v_{j-1})(uv_{j-1} - 1)$ & $\operatorname{div} \mu_p \exp(-\tilde{\psi}_j)\nabla v = \tilde{R}(\tilde{\psi}_j, u_{j-1}, v_{j-1})(u_{j-1}v - 1)$ (+ corresponding boundary conditions). The existence of weak solutions $(H_2(\psi_j, u_{j-1}, v_{j-1}), H_3(\psi_j, u_{j-1}, v_{j-1})) = (u_j, v_j)$ for this system can be deduced from [10, Sec. 3.13, Thm. 13.1], which additionally gives a bound in $L^\infty(\Omega)$ that only depends on the bound corresponding to K for the Dirichlet data and the space dimension. Thanks to the nonnegativity of $\tilde{R}(\tilde{\psi}_j, u_{j-1}, v_{j-1})$ and the bound from below corresponding to the one in* (11) *on the Dirichlet data the maximum principle additionally ensures that (u_j, v_j) are bounded from below by a constant C_1. The $H^1(\Omega)$-bounds ensue from standard coercivity estimates, also using the $L^\infty(\Omega)$-bounds for (u_{j-1}, v_{j-1}) in order to find $\tilde{R}(\tilde{\psi}_j, u_{j-1}, v_{j-1})$ bounded. Hence, one can define a fixed point map $H = (H_1, H_2, H_3) : N \to N$ on the closed, convex set $N = \{(\tilde{\psi}, u, v) \in [L^2(\Omega)]^3,\ C_1 \le u, v \le C_2, |\tilde{\psi}| \le C_3$ a.e. in $\Omega\}$, where the constants C_1, C_2, C_3 correspond to $1/L, L$. Then $\rho_{\mathrm{vR}}(\xi_{\mathrm{D}}; \psi, n, p) = \mathbf{0}$ text if $H(\tilde{\psi}, u, v) = (\tilde{\psi}, u, v)$. Thanks to the above observations on the boundedness of the solutions $(\tilde{\psi}_j, u_j, v_j) \in [H^1(\Omega) \cap L^\infty(\Omega)]^3$, $j \in \mathbb{N}$, one obtains that $H(N) \subset [H^1(\Omega) \cap L^\infty(\Omega)]^3$ is contained in a compact subset of $L^2(\Omega)^3$. Moreover, from the well-posedness of the above elliptic boundary value problems it follows that the solution operator is continuous on $[L^2(\Omega)]^3$. Thus, the existence of a fixed point $H(\tilde{\psi}, u, v) = (\tilde{\psi}, u, v)$ follows by Schauder's fixed point theorem.*

4 Optimization problem

Our optimization goal is to maximize the optical output, i.e. the number of photons available in the device, with respect to the doping profile $C \in \mathbf{C}$ injected into a device, whose electrical properties are governed by the van Roosbroeck system (10). This will amount to a constrained minimization problem for a suitable cost functional $\mathcal{Q} : \mathbf{X} \times \mathbf{C} \to \mathbb{R} \cup \{\infty\}$ which shall be introduced now. Following [2], the optical output is related to the modal net-gain

$$-Q_1(n, p) = (g - \ell)|\Psi|^2, \tag{15}$$

with the representation of the optical mode $\Psi \in C_0^\infty(\Omega)$ as in (6) and with the material gain g and the optical losses ℓ from (4). In view of this, we introduce the functional

$$\widetilde{\mathcal{Q}}_1 : \mathbf{X} \to \mathbb{R}, \quad \widetilde{\mathcal{Q}}_1(\psi, n, p) := \int_\Omega Q_1(\psi + \psi_{\mathrm{D}}, n + n_{\mathrm{D}}, p + p_{\mathrm{D}})\, \mathrm{d}x\,, \tag{16}$$

so that the maximization of the optical output will be realized by minimizing a functional that involves $\widetilde{\mathcal{Q}}_1$. In particular, since the doping profile $C \in \mathbf{C}$ shall be the control parameter of the optimization problem, we shall combine $\widetilde{\mathcal{Q}}_1$ with a second functional

$$\widetilde{\mathcal{Q}}_2 : \mathbf{C} \to \mathbb{R} \cup \{\infty\} \text{ with domain } \operatorname{dom} \widetilde{\mathcal{Q}}_2 = \mathbf{C}_0 \subset \mathbf{C} \text{ a closed, convex subset} \tag{17a}$$

and we impose that $\widetilde{\mathcal{Q}}_2 : \mathbf{C} \to \mathbb{R} \cup \{\infty\}$ is:

- weakly sequentially lower semicontinuous on $\mathbf{C}$, (17b)
- bounded from below and coercive: $\exists\, c_{\mathcal{Q}_2}, \bar{c}_{\mathcal{Q}_2} > 0,\ r \in (1, \infty)$,

$$\forall\, C \in \mathbf{C} :\ \widetilde{\mathcal{Q}}_2(C) \geq c_{\mathcal{Q}_2} \|C\|^r_{\mathrm{C}} - \bar{c}_{\mathcal{Q}_2}. \tag{17c}$$

Making use of (14), (16), and (17a) we finally introduce the cost functional

$$\mathcal{Q} : \mathbf{X}\times\mathbf{C} \to \mathbb{R}\cup\{\infty\},\ \mathcal{Q}(\psi, n, p, C) := \begin{cases} \widetilde{\mathcal{Q}}_1(\psi, n, p) + \widetilde{\mathcal{Q}}_2(C) & \text{if } (\psi, n, p, C) \in \mathbf{S}_{\mathrm{vR}}, \\ \infty & \text{otherwise} \end{cases} \tag{18}$$

and in what follows we shall treat the constrained minimization problem

$$\min_{\mathbf{X}\times\mathbf{C}} \mathcal{Q}(\psi, n, p, C)\,. \tag{19}$$

Observe that the functional $\widetilde{\mathcal{Q}} := \widetilde{\mathcal{Q}}_1 + \widetilde{\mathcal{Q}}_2 : \mathbf{X}\times\mathbf{C} \to \mathbb{R}\cup\{\infty\}$ only carries the compactness property (17c) encoded in $\widetilde{\mathcal{Q}}_2$ for the doping profiles, whereas $\widetilde{\mathcal{Q}}_1$ does not give any compactness for the densities. Therefore it is important to note that the functional $\mathcal{Q}$ gives this missing compactness by constraining the minimization to the set $\mathbf{S}_{\mathrm{vR}}$, which is compact by Prop. 1. This idea will be used in order to prove the existence of a minimizer in (19). In particular, we now collect the following properties of the functional $\mathcal{Q}$:

Proposition 2 (Properties of $\mathcal{Q}$)**.** *The functional $\mathcal{Q} : \mathbf{X} \times \mathbf{C} \to \mathbb{R} \cup \{\infty\}$, defined by the relations* (14)*,* (4a)–(18)*, enjoys the following properties:*

- *$\mathcal{Q}$ is bounded from below and coercive:* $\exists\, C_{\mathcal{Q}_1} \in (-\infty, 0),\ \exists\, c_{\mathcal{Q}_2}, \bar{c}_{\mathcal{Q}_2} > 0, r \in (1, \infty)$,

$$\forall\, (\psi, n, p, C) \in \mathbf{X} \times \mathbf{C} : \mathcal{Q}(\psi, n, p, C) \geq C_{\mathcal{Q}_1} + c_{\mathcal{Q}_2} \|C\|^r_{\mathbf{C}} - \bar{c}_{\mathcal{Q}_2}\,. \tag{20a}$$

- *$\mathcal{Q}$ is lower semicontinuous wrt. convergence in τ_{vR}* . (20b)

Proof: Ad boundedness from below and coercivity (20a)**:** For this, we first check that the density $Q_1 = -(g - \ell)$ is bounded from below. Indeed, for any $n, p > 0$ observe by Young's inequality that $-g(n, p) > -g_0(np)^\delta \geq -\frac{g_0}{2}(n^{2\delta} + p^{2\delta}) =: f(n, p)$. On the interval $[0, \infty)$ the function $F(n, p) := f(n, p) + \ell(n, p)$ has a global minimum at $(n_*, p_*) := \big((\frac{2\delta g_0}{f_{\mathrm{n}}})^{1/(1-2\delta)}, (\frac{2\delta g_0}{f_{\mathrm{p}}})^{1/(1-2\delta)}\big)$ since the Hessian $\mathrm{D}^2 F(n_*, p_*) = -(2\delta{-}1)(2\delta) g_0^2 \operatorname{diag}(n_*^{2\delta-2}, p_*^{2\delta-2})$ is positively definite because of $\delta < 1/2$. This yields that

$$-g(n, p) + \ell(n, p) > F(n, p) \geq F(n_*, p_*) \qquad \text{for any } (n, p) \in [0, \infty)^2\,, \tag{21}$$

hence a bound from below on $\widetilde{\mathcal{Q}}_1$. In combination with the bound (17c) on $\widetilde{\mathcal{Q}}_2$ we thus obtain

$$\mathcal{Q}(\psi, n, p, C) \geq F(n_*, p_*)\mathcal{L}^d(\Omega) + c_{\mathcal{Q}_2} \|C\|^r_{\mathbf{C}} - \bar{c}_{\mathcal{Q}_2}\,.$$

Ad lower semicontinuity (20b)**:** Consider a sequence $(\psi_k, n_k, p_k, C_k) \overset{\tau_{\rm vR}}{\to} (\psi, n, p, C)$. In the case that $(\psi_k, n_k, p_k, C_k) \in (\mathbf{X} \times \mathbf{C}) \backslash \mathbf{S}_{\rm vR}$ for all but a finite number of indices, then there is nothing to check because $\infty = \liminf_{k\to\infty} \mathcal{Q}(\psi_k, n_k, p_k, C_k) \geq \mathcal{Q}(\psi, n, p, C)$. Assume that $(\psi_k, n_k, p_k, C_k)_k \subset \mathbf{S}_{\rm vR}$ for a not relabelled subsequence. By the compactness of $\mathbf{S}_{\rm vR}$, ensured by Prop. 1, we thus find that the limit $(\psi, n, p, C) \in \mathbf{S}_{\rm vR}$. Therefore we may argue that the lower semicontinuity estimate for $\mathcal{Q}$ in this case coincides with the lower semicontinuity of $\widetilde{\mathcal{Q}}_1 + \widetilde{\mathcal{Q}}_2$. Then, $\liminf_{k\to\infty} \widetilde{\mathcal{Q}}_2(C_k) \geq \widetilde{\mathcal{Q}}(C)$ by (17b). We now check that $\widetilde{\mathcal{Q}}_1$ is lower semicontinuous with respect to strong convergence of $(n_k, p_k)_k$ in $L^q(\Omega) \times L^q(\Omega)$ for any $q \in (1, \infty)$, which corresponds to convergence property 3 in (13). For this, we use that $-g(n_k, p_k) + \ell(n_k, p_k) > F(n_*, p_*)$, which serves as an integrable minorant according to (21), since in particular $(n_*, p_*) = \big((\frac{2\delta g_0}{f_n})^{1/(1-2\delta)}, (\frac{2\delta g_0}{f_p})^{1/(1-2\delta)}\big) \in L^q(\Omega) \times L^q(\Omega)$ for any $q \in [1, \infty]$. Moreover, since strong L^q-convergence implies the convergence of the sequence in measure, Fatou's lemma ultimately yields the lower semicontinuity. ■

The existence of a minimizer can now immediately be concluded by employing the direct method of the calculus of variations, making use of the boundedness from below, the coercivity of $\mathcal{Q}$ and its lower semicontinuity.

Theorem 2 (Existence of minimizers for the constrained minimization problem)**.** *Let the functional* $\mathcal{Q} : \mathbf{X} \times \mathbf{C} \to \mathbb{R} \cup \{\infty\}$ *be defined by* (4a)*,* (14)*,* (15)*–*(18)*. Then the constrained minimization problem* (19) *admits at least one solution* $(\psi, n, p, C) \in (\mathbf{X} \times \mathbf{C}) \cap \mathbf{S}_{\rm vR}$*.*

Remark 3 (Different choices of $\mathbf{C}$ and $\mathcal{Q}_2$)**.** *If* $\mathbf{C} = H^1(\Omega)$*, possible choices for* $\mathcal{Q}_2$ *are e.g.* $\mathcal{Q}_2^{\rm D}$ *or* $\mathcal{Q}_2^{\rm N}$ *defined by*

$$\mathcal{Q}_2^{\rm D}(C) := \begin{cases} \frac{\gamma}{2}\|\nabla(C + C_{\rm D} - \bar{C})\|^2_{L^2(\Omega)} & \text{if } C \in H^1_{\rm D}(\Omega), \\ \infty & \text{otherwise}, \end{cases} \tag{22a}$$

$$\mathcal{Q}_2^{\rm N}(C) := \begin{cases} \frac{\gamma}{2}\|C - \bar{C}\|^2_{H^1(\Omega)} & \text{if } C \in H^1(\Omega), \\ \infty & \text{otherwise}, \end{cases} \tag{22b}$$

where $\gamma > 0$ *is a weight,* $\bar{C} \in H^1(\Omega)$ *is a given "desired" doping profile and* $C_{\rm D} \in H^1(\Omega) \cap L^\infty(\Omega)$ *the extension of a given Dirichlet datum into the domain. Note that in the first case a Poincaré inequality is available to ensure the boundedness from below* (17c) *in terms of the full* $H^1(\Omega)$*-norm.*

If $\mathbf{C} = H^1(\Omega)$*, the traces to the boundary are well-defined for the doping profile* C*. Then also the Dirichlet boundary conditions for* (ψ, n, p) *can be formulated in terms of the corresponding boundary datum of* C*, thus allowing for Ohmic contacts* (1c)*, cf. [4, 7], where the built-in potential* $\psi_{\rm bi}$ *is determined by*

$$C_{\rm D} + n_i(e^{-\psi_{\rm bi}} - e^{\psi_{\rm bi}}) = 0, \qquad \text{on } \Gamma_{\rm D}. \tag{23}$$

which results in $n_{\rm D} = \big(C_{\rm D} + (C_{\rm D}^2 + 4n_i^2)^{1/2}\big)/2$ *and* $p_{\rm D} = C_{\rm D} - n_{\rm D}$*. Hence, in case of* (22a) *one has to ensure that* $\max\{(\frac{1}{K} - Kn_i), (\frac{n_i}{K} - K)\} \leq C_{\rm D} \leq \min\{(K - \frac{n_i}{K}), (n_iK - \frac{1}{K})\}$*, in order to match* (3) *with* (11)*. In case of* (22b) *condition* (11) *is harder to meet as one has to additionally impose that* $C \in L^\infty(\Gamma_{\rm D})$*. This can be achieved either by adding a further suitable penalization term to* $\mathcal{Q}_2^{\rm N}$ *or, as we will do in Sec. 4, by treating the problem* *in space dimension $d = 1$, where $H^1(\Omega)$ compactly embeds into $C(\overline{\Omega})$, i.e. $\|C\|_{C(\overline{\Omega})} \leq c\|C\|_{\mathbf{C}} =: Z$. For this latter case we find with $K(\|C\|_{\mathbf{C}}) := \max\{m(C), M(C)\}$, where $m(C) := (\min_{z\in[0,Z]}\{n_{\mathrm{D}}(z), p_{\mathrm{D}}(z)\})^{-1}$, and $M(C) = \max_{z\in[0,Z]}\{n_{\mathrm{D}}(z), p_{\mathrm{D}}(z), \psi_{\mathrm{D}}(z)\}$ that $K(\|C\|_{\mathbf{C}})^{-1} \leq n_{\mathrm{D}}(C), p_{\mathrm{D}}(C) \leq K(\|C\|_{\mathbf{C}})$ as well as $\|\psi_{\mathrm{D}}(C)\|_{L^\infty(\Omega)} \leq K(\|C\|_{\mathbf{C}})$. Thus, for the data $(n_{\mathrm{D}}(C), p_{\mathrm{D}}(C), \psi_{\mathrm{D}}(C))$ from* (3) *in* (10) *one has $K = K(\|C\|_{\mathbf{C}})$ in* (11) *and hence, $L = L(\Omega, K(\|C\|_{\mathbf{C}}), \|C\|_{\mathbf{C}})$. According to Remark 2, thanks to the continuous dependence of L on its parameters, both constants are bounded on bounded sets in $\mathbf{C}$. Hence, it remains true that $\mathbf{S}_{\mathrm{vR}}$ is compact in $\mathbf{X} \times \mathbf{C}$ with respect to τ_{vR}.*

In the case $\mathbf{C} = L^p(\Omega)$ a possible choice of $\mathcal{Q}_2$ would be

$$\mathcal{Q}_p^{\mathrm{L}}(C) = \begin{cases} \frac{\gamma}{2}\|C - \bar{C}\|^p_{L^p(\Omega)} & \text{if } C \in L^p(\Omega), \\ \infty & \text{otherwise}, \end{cases} \tag{24}$$

where traces are generally not well-defined. In this case we adopt artificial Ohmic contacts by defining the built-in potential as

$$\bar{C} + n_i(e^{-\psi_{\mathrm{bi}}} - e^{\psi_{\mathrm{bi}}}) = 0, \qquad \text{on } \Gamma_{\mathrm{D}}. \tag{25}$$

This choice is not driven by any physical meaning but in order to study its impact on optimized doping profiles. In particular for $\gamma \to 0$ the artificial Ohmic contact will in general strongly violate the desired charge-neutrality.

Remark 4 (The first order optimality system)**.** *In the following we assume that*

$$\operatorname{dom} \widetilde{\mathcal{Q}}_2 = \mathbf{C} \text{ and } \widetilde{\mathcal{Q}}_2 : \mathbf{C} \to \mathbb{R} \text{ is twice continuously Fréchet differentiable.} \tag{26}$$

Observe that $\widetilde{\mathcal{Q}}_1 : \mathbf{X} \to \mathbb{R}$ is indeed twice continuously Fréchet differentiable. In this way, the cost functional $\widetilde{\mathcal{Q}} = \widetilde{\mathcal{Q}}_1 + \widetilde{\mathcal{Q}}_2 : \mathbf{X} \times \mathbf{C} \to \mathbb{R}$ satifies the assumptions posed in [7, Sec.s 3,4] and hence the first order optimality system and the existence of Lagrange multipliers can be obtained following the lines of [7, Sec. 4]. Abbreviating $\xi := (\psi, n, p)$, we write the Lagrangian associated to the minimization problem (19)

$$\mathcal{L}_{\mathrm{vR}} : \mathbf{X} \times \mathbf{C} \times \mathbf{H} \to \mathbb{R}\,,\ \mathcal{L}_{\mathrm{vR}}(\xi, C, \lambda) := \widetilde{\mathcal{Q}}(\xi, C) + \langle \rho_{\mathrm{vR}}(\xi_{\mathrm{D}}; \xi, C), \lambda\rangle_{\mathbf{H}}\,. \tag{27}$$

The associated first order optimality condition reads $\mathrm{D}_{(\xi,C,\lambda)}\mathcal{L}_{\mathrm{vR}}(\xi, C, \lambda) = \mathbf{0}$ in $\mathbf{X}^* \times \mathbf{C}^* \times \mathbf{H}^*$. The existence and uniqueness of a Lagrange multiplier λ is verified in [7, Thm. 4.2] under an additional smallness condition on the quotients j_n^2/n and j_p^2/p. For Ohmic contacts as in (3) *and* (23) *the derivative $\mathrm{D}_C\mathcal{L}_{\mathrm{vR}}$ also acts on the dependence of ξ_{D} on C at Γ_{D}.*

5 Numerical results

The numerics is based on a stationary formulation of (1) in terms of the original quasi-Fermi potentials φ_n, φ_p introduced in (1b) and the electrostatic potential ψ in one spatial dimension. Unlike the standard approach by Scharfetter-Gummel schemes [14], we use finite differences on a mesh $0 = x_1 < \ldots < x_k < \ldots < x_N = 1$ where the discrete electron current is expressed using $\varphi_{n;k} = \varphi_n(x_k)$, $\varphi_{p;k} = \varphi_p(x_k)$, $\psi_k = \psi(x_k)$, $\eta_{p;k} = (\varphi_{p;k} - \psi_k)$ and $\eta_{n;k} = (\psi_k - \varphi_{n;k})$ as

$$\mathrm{j}_{n;k+1/2} = -\mu_n n_i \exp\left(\tfrac{1}{2}(\eta_{n;k+1} + \eta_{n;k})\right) \left(\frac{\varphi_{n;k+1} - \varphi_{n;k}}{x_{k+1} - x_k}\right),$$
$$\mathrm{j}_{p;k+1/2} = -\mu_p n_i \exp\left(\tfrac{1}{2}(\eta_{p;k+1} + \eta_{p;k})\right) \left(\frac{\varphi_{p;k+1} - \varphi_{p;k}}{x_{k+1} - x_k}\right),$$

and approximate the divergence by $\partial_x j_n \approx (\mathrm{j}_{n;k+1/2} - \mathrm{j}_{n;k-1/2})/(x_{k+1/2} - x_{k-1/2})$. The hole current $j_p = -\mu_p p \partial_x \varphi_p$ is discretized analogously. For sake of notation we use $\xi = (\psi, \varphi_n, \varphi_p)^\top$. Introducing the flux $j_{\psi;k+1/2} = -(\psi_{k+1} - \psi_k)/(x_{k+1} - x_k)$ the previous expressions can be combined into the following discrete and nonlinear residual $\widetilde{\rho}_{\mathrm{vR}} : \mathbb{R}^{3N} \times \mathbb{R}^N \to \mathbb{R}^{3N}$ as

$$\widetilde{\rho}_{\mathrm{vR}}(\xi, C) = \begin{pmatrix} \frac{\mathrm{j}_{\psi;k+1/2} - \mathrm{j}_{\psi;k-1/2}}{x_{k+1/2} - x_{k-1/2}} - \widehat{Q}_k \\ \frac{\mathrm{j}_{n;k+1/2} - \mathrm{j}_{n;k-1/2}}{x_{k+1/2} - x_{k-1/2}} - R_k \\ \frac{\mathrm{j}_{p;k+1/2} - \mathrm{j}_{p;k-1/2}}{x_{k+1/2} - x_{k-1/2}} + R_k \end{pmatrix}$$

for $k = 2, ..., N-1$ and with the total charge $\widehat{Q}_k(\xi, C) = q\big(C_k + n_i \exp(\eta_{p;k}) - n_i \exp(\eta_{n;k})\big)$. This residual is the equivalent to the operator introducted in (9). It depends on the doping through the total charge and through the boundary conditions. The boundary conditions (1c) in $\widetilde{\rho}_{\mathrm{vR}}$ for $k = 1$ and $k = N$ are $\psi_k = \psi_{\mathrm{bi}}(C_k) + \psi_{\mathrm{ext};k}$ and $\varphi_{n/p;k} = \psi_{\mathrm{ext};k}$. The discretized van Roosbroeck equation, which now reads $\widetilde{\rho}_{\mathrm{vR}}(\xi, C) = \mathbf{0}$, is then solved using a Newton method $\xi^{n+1} = \xi^n - (\partial_\xi \widetilde{\rho}_{\mathrm{vR}})^{-1} \widetilde{\rho}_{\mathrm{vR}}$. In thermal equilibrium $\psi_{\mathrm{ext}} = 0$ we have $\varphi_n = \varphi_p \equiv 0$, so that since $q \gg 1$ it makes sense to choose $\xi^0 = (\psi^0, 0, 0)^\top$ with ψ^0 so that $\widehat{Q}_k = q\big(C_k + n_i(e^{-\psi_k^0} - e^{\psi_k^0})\big) = 0$. As the magnitude of the bias ψ_{ext} is increased, the previous solution with smaller bias is used as the starting-point for the Newton method.

For the present paper the recombination in (7) is $\tilde{R} = (C_n n + C_p p) + (\tau_p(n + n_i) + \tau_n(p + n_i))^{-1}$, with the parameters $C_n = C_p = 10^{-1}$, $\tau_n = \tau_p = 10$, $n_i = 10^{-2}$. Additionally we have $q = 10^2$, $\mu_n = \mu_p = 1$. The external potential is $\varphi_{\mathrm{ext}} = 0.4\,\mathrm{V}/U_T \approx 15.47$ for $T = 300\,\mathrm{K}$. These values are somewhat realistic in the sense that usually one has $0 < n_i \ll 1$ and $q \gg 1$. The optical mode is set to a Gaussian $|\Psi|^2 = \exp\big(-(10(x - 1/2))^2\big)$ and the parameters in the net-gain (4) are $f_n = 1/5$, $f_p = 1$, $\delta = 0.3$, $g_0 = e^{-1}$, $g_1 = n_i^2$.

The optimization strategy for (19) is similar to [8], where we discretize the cost functional $\mathcal{Q}_1$ by

$$\mathcal{Q}_1(\xi) = \sum_{k=1}^{N} h\, Q_1(n_k, p_k), \tag{28a}$$

with $Q_1 = -\big(g(n_k, p_k) - \ell_k\big)|\Psi_k|^2$ and free-carrier absorbtion $\ell_k = f_{\mathrm{n}} n_k + f_{\mathrm{p}} p_k$.

The different regularization terms $\mathcal{Q}_2^{\mathrm{N/D}}$ from (22) for $\mathbf{C} = H^1(\Omega)$ or $\mathbf{C} = H_0^1(\Omega)$ are treated equally within our discretization by a functional $\mathcal{Q}_2$. Together with the functional $\mathcal{Q}_2^{\mathrm{L}}$ for $\mathbf{C} = L^2(\Omega)$ we discretize using

$$\mathcal{Q}_2(C) = \frac{\gamma}{2} \sum_{k=1}^{N-1} h \left(\frac{C_{k+1} - C_k + \bar{C}_{k+1} - \bar{C}_k}{h}\right)^2, \qquad \mathcal{Q}_2^{\mathrm{L}}(C) = \frac{\gamma}{2} \sum_{k=1}^{N} h \left(C_k - \bar{C}_k\right)^2 \tag{28b}$$

where $h = x_{k+1} - x_k$, which for this paper we assume to be constant. Note that for $\mathcal{Q}_2^{\mathrm{N}}$ from (22b) the boundary values for C are not kept fixed. Hence, (22b) suggests to use the full $H^1(\Omega)$-norm for regularization. However, here we study the effect of different regularizations and thereby use the $L^2(\Omega)$-norm and $H^1(\Omega)$-seminorm separately. As before we use $\tilde{\mathcal{Q}}(\xi, C) = \mathcal{Q}_1(\xi) + \mathcal{Q}_2(C)$ and introduce a Lagrange multiplier $\lambda \in \mathbb{R}^n$, so that the first-order optimality conditions using the discrete counterpart $\mathcal{L}_{\mathrm{vR}} : \mathbb{R}^{3N} \times \mathbb{R}^{\hat{N}} \times \mathbb{R}^{3N} \to \mathbb{R}$ of the Lagrangian in (27) is $\mathcal{L}'_{\mathrm{vR}} = (\mathcal{L}_{\mathrm{vR},\xi}, \mathcal{L}_{\mathrm{vR},C}, \mathcal{L}_{\mathrm{vR},\lambda}) = 0$. For $\langle u, v\rangle$ we use the standard inner product in $\mathbb{R}^{3N}$. Note that, unlike [8], $\widetilde{\rho}_{\mathrm{vR}}$ is not linear in C, if we do not fix the value of C_1, C_N. In this case $\hat{N} = N$, otherwise $\hat{N} = N - 2$. Due to the nonlinearity of the boundary conditions (23) in C, this produces the slightly different reduced Hessian $\hat{\mathcal{Q}}''$ of $\hat{\mathcal{Q}}(C) = \mathcal{Q}(\xi(C), C)$ being

$$\hat{\mathcal{Q}}'' = \mathcal{Q}_{,CC} + \langle \tilde{\rho}_{\mathrm{vR,CC}}, \lambda \rangle + \tilde{\rho}^{*}_{\mathrm{vR,C}} \tilde{\rho}^{-*}_{\mathrm{vR},\lambda} \left[Q_{,\xi\xi} + \langle \tilde{\rho}_{\mathrm{vR},\xi\xi}, \lambda \rangle \right] \tilde{\rho}^{-1}_{\mathrm{vR},\xi} \tilde{\rho}_{\mathrm{vR,C}} \in \mathbb{R}^{\hat{N} \times \hat{N}}.$$

As in [8] we have an outer Newton iteration $C^{r+1} = C^r + \delta C^r$, which utilizes an inner CG iteration in order to solve $\hat{\mathcal{Q}}''(C^r)\delta C^r = -\hat{\mathcal{Q}}'(C^r)$.

The primary question in designing a realistic optoelectronic optimization problem is to find a cost functional, which combines the desired optimality with mathematical simplicity. Furthermore the cost functional should be feasible from a optimization point of view, for which it might be necessary to add regularizing terms to the cost. Here we study the influence of such regularizing terms $\mathcal{Q}_2$ in (28b) of tracking type on the optimal solution. We study the influence of tracking the values in $L^2(\Omega)$ or the gradients in $H^1(\Omega)$ with respect to a reference doping $\bar{C}$. Furthermore we study the influence of the corresponding regularization parameter γ and the boundary condition on the control space $\mathbf{C}$.

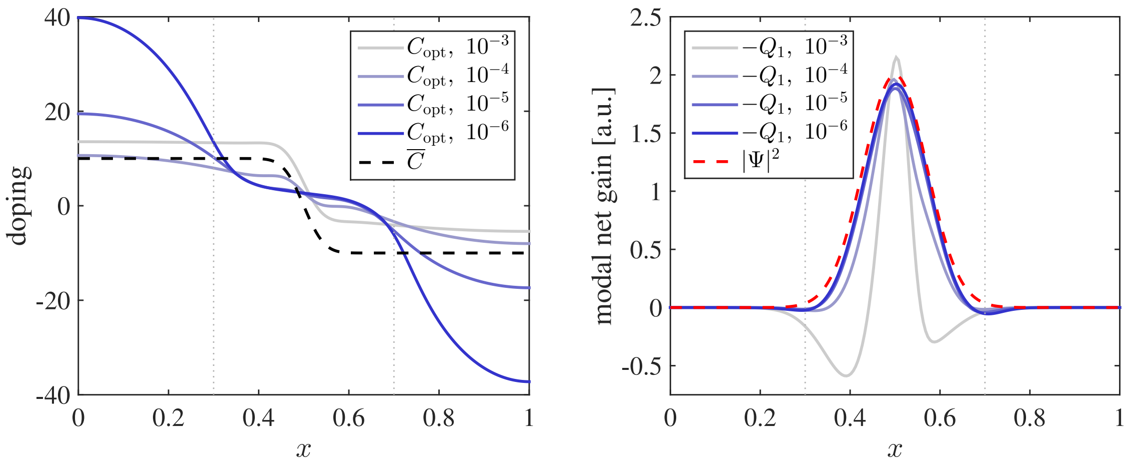

Figure 1: (Left) optimal doping densities C_{opt} for different regularization parameters γ and reference doping $\bar{C}$ and (Right) corresponding modal net gain $-Q_1 = (g - \ell)|\Psi|^2$ compared to mode intensity $|\Psi|^2$ (arbitrary scaling). The values of the cost functional are $\mathcal{Q}_1 = \{0.05, 0.25, 0.30, 0.31\}$ for $\gamma = \{10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}\}$ and $\mathcal{Q}_1 = -0.24$ for $C = \bar{C}$

In the left panel of Fig. 1 we show the optimal doping C_{opt} for various regularization parameters γ for gradient regularization without a fixed boundary condition, i.e. the case of $H^1_0(\Omega)$. As

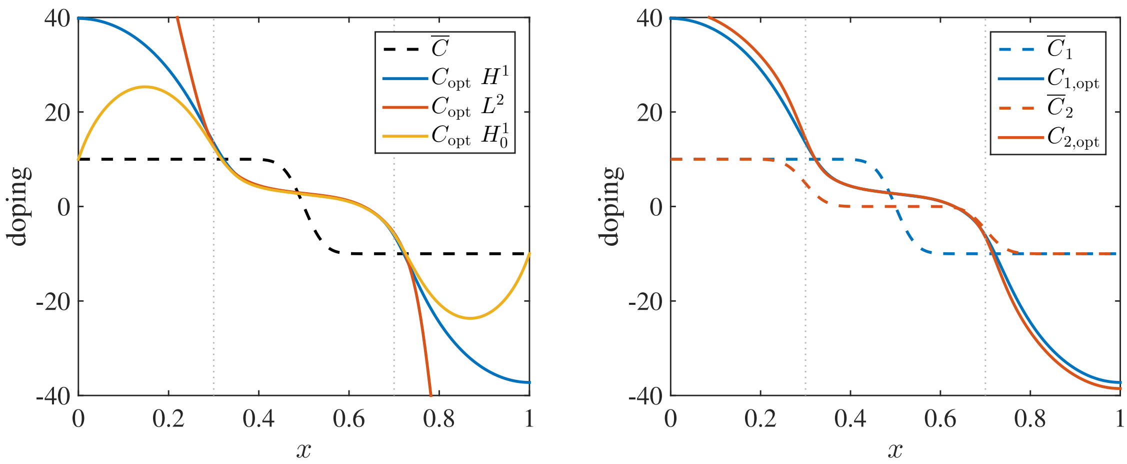

Figure 2: (Left) optimal doping densities C_{opt} for different regularization functionals and spaces $H^1(\Omega), H^1_0(\Omega), L^2(\Omega)$ for $\gamma = 10^{-6}$ and reference doping $\bar{C}$ and (Right) optimal doping densities C_{opt} for $\gamma = 10^{-6}$ and two different reference dopings $\bar{C}_1 = 10\tanh\big(25(\frac{1}{2} - x)\big)$ and $\bar{C}_2 = 5\tanh\big(25(0.3 - x)\big) + 5\tanh\big(25(0.7 - x)\big)$

$\gamma \to 0$ we observe that the optimal solution stabilizes/converges where the major part of the support of $|\Psi|^2$ is located (as indicated by the dotted light gray vertical lines), whereas the doping still increases where $|\Psi|^2 \simeq 0$. For larger regularization parameters $\gamma > 10^{-5}$ the shape is still affected by the single-step reference doping, whereas for smaller regularization parameters there is very little dependence on the reference. At the same time one can see that $-Q_1 = (g - \ell)|\Psi|^2$ converges to a mostly positive solution as $\gamma \to 0$, whereas for $\gamma > 10^{-3}$ large parts of $-Q_1$ are still negative.

This can also be observed in Fig. 2. In its left panel the optimal doping is shown for $H^1(\Omega)$ regularization with $\gamma = 10^{-6}$ and two different reference dopings, e.g. a smoothed single-step and a smoothed double-step doping. Where $|\Psi|^2$ is located both optimal dopings agree and where $|\Psi|^2 \simeq 0$ the solutions are close. Even for entirely different regularization, the left panel shows that the optimal dopings are basically the same for $H^1(\Omega)$, $L^2(\Omega)$, and $H^1_0(\Omega)$ regularization. The main effect can be observed near the boundary, where $|\Psi|^2 \simeq 0$. The $L^2(\Omega)$ regularization is only a slight restriction on the doping and hence the solution is largest near the boundaries. In this case also $\mathcal{Q}_2$ is slightly larger than for the $H^1(\Omega)$ regularization, which, in turn, is slightly larger than for the $H^1_0(\Omega)$ regularization. However, since the gains in all three cases are very similar, we can conclude also here that for sufficiently small γ also the influence on Q_1 is very small. We observed that when the regularization parameter is sufficiently small, then the choice of the regularization mechanism has an effect on the optimal solution but only small effect on the optimal gain.

We conclude that, in 1D the choice regularization of the optimization problem has little influence on the optimizer in regions, where the main part of the optical mode is located.

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