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Abstract We derive an optoelectronic model based on a gradient formulation for the relaxation of electron-, hole- and photon-densities to their equilibrium state. This leads to a coupled system of partial and ordinary differential equations, for which we discuss the isothermal and the non-isothermal scenario separately.

1 Introduction

The aim of this work is to formulate a model for opto-electronic processes in semiconductors as a generalized gradient system. We will discuss the isothermal case and the non-isothermal case. For both cases we will consider the admissible state variables $\boldsymbol{q}$ in a state space $\boldsymbol{Q}$, and determine a suitable thermodynamical functional $\Phi : \boldsymbol{Q} \to \mathbb{R}$, that drives all the opto-electronic processes, as well as a potential $\Psi^* : \boldsymbol{Q} \times \boldsymbol{Q}^* \to [0,\infty)$ encoding the different additive dissipative processes in the material. With the aid of these functionals Φ and Ψ^*, the evolution of the state $\boldsymbol{q}$ is governed by the rate equation

$$\dot{\boldsymbol{q}} = \mathrm{D}_{\boldsymbol{\eta}} \Psi^*(\boldsymbol{q}; -\mathrm{D}_{\boldsymbol{q}} \Phi(\boldsymbol{q})) \quad \text{ in } \boldsymbol{Q} \tag{1}$$

where $\dot{\boldsymbol{q}}$ denotes the time-derivative of the state vector $\boldsymbol{q}$ and $\mathrm{D}_{\boldsymbol{\eta}} \Psi^*(\boldsymbol{q}; \boldsymbol{\eta})$ denotes the derivative of $\Psi^*(\boldsymbol{q}; \boldsymbol{\eta})$ wrt. the variable $\boldsymbol{\eta}$, and similarly, $\mathrm{D}_{\boldsymbol{q}} \Phi(\boldsymbol{q})$ the derivative of $\Phi(\boldsymbol{q})$ wrt. $\boldsymbol{q}$.

It was first shown in [10, 11, 5] that certain diffusion processes can be written as gradient flows of the form (1) with Φ given by the free energy or the entropy functional. In [7, 8] it was proven that also *reaction*-diffusion systems can be cast

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in the gradient structure of (1) and in [7, 4] this approach was adapted to the drift-diffusion and recombination processes arising in semiconductors.

In this contribution we will show that also the opto-electronic models treated in, *e.g.*, [13, 12, 2] fall into the framework of (1), see [7, 8, 4]. These models consist of transport equations for the densities of charge carriers, electrons n and holes p, and describe their motion in the device driven by diffusion and drift in a self-consistent electrical field $\boldsymbol{E} = -\nabla\varphi_c$. In addition, electrons, holes and photons are generated or annihilated according to different radiative and non-radiative processes, coupled to the equations in a thermodynamically consistent way. The number of photons generated by such kinds of radiative recombination mechanisms is determined by a photon rate equation, which arises from the corresponding reaction kinetics; this feature so far was not considered in [7, 8, 4].

To incorporate the photon rate equation to our gradient flow formulation we make use of the ideas of [14]. Therein, the key idea is to extend the classical thermodynamic treatment of electromagnetic radiation beyond the purely thermal black-body radiation towards *luminescent radiation* which is observed, *e.g.*, in diodes and lasers. It is assumed that optoelectronic excitations in a semiconductor lead to an equilibrium of electron/hole chemical potentials μ_c, μ_v with the photon chemical potential μ_γ so that $\mu_\gamma = \mu_c + \mu_v$. This leads to a modified radiation formula following Bose-Einstein statistics for the number of photons per volume and energy interval

$$\rho(E)f(E,\mu) = \frac{E^2}{\pi^2}\left(\frac{n_r}{\hbar c}\right)^3\left(\exp\left(\tfrac{E-\mu_\gamma}{k_{\mathrm{B}}\theta}\right)-1\right)^{-1} \approx \frac{E^2}{\pi^2}\left(\frac{n_r}{\hbar c}\right)^3\exp\left(-\tfrac{E-\mu_\gamma}{k_{\mathrm{B}}\theta}\right),$$

with $E = \hbar\omega$ beyond Planck distribution in equilibrium, where $\mu_\gamma \equiv 0$ for photons, *cf.* [14]. From this, by standard thermodynamics, we can compute entropy and energies as functions of photon density γ and temperature θ, *cf.*, [6]. This approach allows us to adapt the framework of [4] to optoelectronics. In order to present simple closed-form expressions in this contribution, we assume that electron-, hole-, and photon-distributions can be approximated by Boltzmann distributions.

2 Gradient structure: From functionals to differential equations

Thermodynamic functionals. The optoelectronic system consists of negatively charged electrons n in the conduction band and positively charged holes p in the valence band. The density of states is parabolic with band edges $E_{\mathrm{c}}, E_{\mathrm{v}}$ and effective masses m_c^*, m_v^* for conduction and valence band. Furthermore we have a photon density γ in the system with constant refractive index n_r and quadratic density of states. While the electron and hole densities n, p are space-dependent, it is assumed that the photon density γ is constant in space. This leads to the following effective densities of state for electrons (conduction band), holes (valence band), and photons in equilibrium

$$\bar{n} = N_{\mathrm{c}} = 2\left(\tfrac{m_c^* k_{\mathrm{B}}\theta}{2\pi\hbar^2}\right)^{3/2}, \quad \bar{p} = N_{\mathrm{v}} = 2\left(\tfrac{m_v^* k_{\mathrm{B}}\theta}{2\pi\hbar^2}\right)^{3/2}, \quad \bar{\gamma} = \tfrac{2}{\pi^2}\left(\tfrac{n_r k_{\mathrm{B}}\theta}{\hbar c}\right)^3, \qquad (2)$$

and to the intrinsic carrier density $n_i^2 = \bar{n}\bar{p}\exp\big((E_\mathrm{v}-E_\mathrm{c})/(k_\mathrm{B}\theta)\big)$. In (2) by $\hbar$ we denote the Dirac constant, k_B is the Boltzmann constant, and θ is the absolute temperature. We use the notation $\boldsymbol{c} = (c_1,c_2,c_3) = (n,p,\gamma)$ and $\bar{\boldsymbol{c}} = (\bar{c}_1,\bar{c}_2,\bar{c}_3) = (\bar{n},\bar{p},\bar{\gamma})$, where all $c_i,\bar{c}_i$ are densities with units of $(\text{length})^{-3}$. Assuming the Boltzmann distributions for charge carriers and photons, we define the internal energy $\mathscr{U}$, the entropy $\mathscr{S}$, and the free energy $\mathscr{F}$ of the system as

$$\mathscr{U}(\boldsymbol{c},\theta) = \int_\Omega U\,\mathrm{d}x, \qquad \mathscr{S}(\boldsymbol{c},\theta) = \int_\Omega S\,\mathrm{d}x, \qquad \mathscr{F}(\boldsymbol{c},\theta) = \int_\Omega F\,\mathrm{d}x, \tag{3a}$$

where $\Omega \subset \mathbb{R}^3$ is an open bounded domain occupied by the semiconductor. Moreover, $F(\boldsymbol{c},\theta) = U(\boldsymbol{c},\theta) - \theta S(\boldsymbol{c},\theta)$, where the densities U and S are given by

$$U(\boldsymbol{c},\theta) = \frac{\varepsilon}{2}|\nabla\varphi_c|^2 + k_\mathrm{B}\theta\left(\tfrac{3}{2}(n+p)+3\gamma\right) + E_\mathrm{c}n - E_\mathrm{v}p + c_V\theta, \tag{3b}$$

$$S(\boldsymbol{c},\theta) = -k_\mathrm{B}\left[n\left(\log\tfrac{n}{\bar{n}} - \tfrac{5}{2}\right) + p\left(\log\tfrac{p}{\bar{p}} - \tfrac{5}{2}\right) + \gamma\left(\log\tfrac{\gamma}{\bar{\gamma}} - 4\right)\right] + c_V\log\theta, \tag{3c}$$

in which $c_V\theta$ and $c_V\log\theta$ constitute lattice contributions to the internal energy in (3b) and the entropy in (3c), where c_V denotes the heat capacity of the lattice. The contribution to the entropy by electrons and holes are given by the Sackur-Tetrode equation. The internal energy density U in (3b) contains the electrostatic potential φ_c, which depends implicitly on $\boldsymbol{c}$ as it is determined by the Poisson equation

$$-\nabla\cdot\varepsilon\nabla\varphi_c = e(C+p-n), \tag{3d}$$

where C is the given concentration of dopants, e is the elementary charge and ε denotes the dielectric permittivity. Now we define dual dissipation functionals $\Psi^*(\boldsymbol{q};\boldsymbol{\eta}) = \Psi^*_\mathrm{rec}(\boldsymbol{q};\boldsymbol{\eta}) + \Psi^*_\mathrm{diff}(\boldsymbol{q};\boldsymbol{\eta})$, for which we separately discuss additive contributions due to recombinations and diffusion.

Dissipation by recombinations with detailed balance. Between electrons, holes, and photons we consider different types of recombinations r with stoichiometric coefficients $\boldsymbol{\alpha}^r = (\alpha_1^r,\alpha_2^r,\alpha_3^r)$ and $\boldsymbol{\beta}^r = (\beta_1^r,\beta_2^r,\beta_3^r)$ in the sense of [7]. As can be found in, *e.g.*, [2, 12, 3] recombinations, characteristic for optoelectronic semiconductor materials, can be written in the form

$$\alpha_1^r n + \alpha_2^r p + \alpha_3^r\gamma \underset{k_-^r}{\overset{k_+^r}{\rightleftharpoons}} \beta_1^r n + \beta_2^r p + \beta_3^r\gamma.$$

In particular, this form includes non-radiative recombination-generation processes such as Auger- and Shockley-Read-Hall, as well as radiative emission-absorption, both spontaneous and stimulated. More precisely, their specific form is

$$\begin{array}{llll}
n+p \rightleftharpoons \emptyset & \text{thus} & \boldsymbol{\alpha}^1-\boldsymbol{\beta}^1 = (1,1,0)^\top & \text{recombination-generation,}\\
n+p+\gamma \rightleftharpoons 2\gamma & \text{thus} & \boldsymbol{\alpha}^2-\boldsymbol{\beta}^2 = (1,1,-1)^\top & \text{stimulated absorption-emission,}\\
n+p \rightleftharpoons \gamma & \text{thus} & \boldsymbol{\alpha}^3-\boldsymbol{\beta}^3 = (1,1,-1)^\top & \text{spontaneous absorption-emission,}
\end{array}$$

each of them with forward reaction rate k_+^r and backward reaction rate k_-^r. Assuming detailed balance there is a steady state $\hat{\boldsymbol{c}}$ so that $k_r(\boldsymbol{q}) = k_+^r(\boldsymbol{q})\hat{\boldsymbol{c}}^{\boldsymbol{\alpha}^r} = k_-^r(\boldsymbol{q})\hat{\boldsymbol{c}}^{\boldsymbol{\beta}^r}$. This notation means $\hat{\boldsymbol{c}}^{\boldsymbol{\alpha}^r} = \hat{n}^{\alpha_1^r}\hat{p}^{\alpha_2^r}\hat{\gamma}^{\alpha_3^r}$. Following [7, 8] and using $\widetilde{\boldsymbol{\eta}} = (\eta_n, \eta_p, \eta_\gamma)$ a suitable dual dissipation functional for the recombinations is given by

$$\Psi_{\text{rec}}^*(\boldsymbol{q};\boldsymbol{\eta}) = \int_\Omega \frac{1}{2}\widetilde{\boldsymbol{\eta}} \cdot \mathbb{H}(\boldsymbol{q})\widetilde{\boldsymbol{\eta}}\,\mathrm{d}x, \quad \mathbb{H}(\boldsymbol{q}) = \sum_{r=1}^{3} \Lambda_r(\boldsymbol{q})(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r)\otimes(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r), \tag{4a}$$

$$\Lambda_r(\boldsymbol{q}) = k_r(\boldsymbol{q})\,\ell\left(\left(\frac{\boldsymbol{c}}{\hat{\boldsymbol{c}}}\right)^{\boldsymbol{\alpha}^r}, \left(\frac{\boldsymbol{c}}{\hat{\boldsymbol{c}}}\right)^{\boldsymbol{\beta}^r}\right), \quad \text{where} \quad \ell(x,y) = \begin{cases} \frac{x-y}{\log x - \log y} & x \neq y, \\ y & x = y. \end{cases} \tag{4b}$$

Note that $\mathbb{H}$, defined in (4a), is symmetric by construction and positive semidefinite on the stochiometric subspace (for details see [7]).

Isothermal model. In the isothermal case we have $\boldsymbol{q} = \boldsymbol{c}$ and the gradient dynamics with fixed $\theta = \theta_\star$, is driven by the free energy $\mathscr{F}(\boldsymbol{c}) \equiv \mathscr{F}(\boldsymbol{c}, \theta_\star)$, so that the evolution of the state variables $\boldsymbol{q} = \boldsymbol{c}$ is given by $\dot{\boldsymbol{c}} = \mathrm{D}_{\boldsymbol{\eta}}\Psi^*\big(\boldsymbol{c}; -\mathrm{D}\mathscr{F}(\boldsymbol{c})\big)$. Using a projector $\mathrm{P} \in \mathbb{R}^{2\times 3}$ such that $\mathrm{P}\boldsymbol{\eta} = (\eta_n, \eta_p)^\top$, we introduce the dual dissipation potential for diffusion as follows

$$\Psi_{\text{diff}}^*(\boldsymbol{q};\boldsymbol{\eta}) = \int_\Omega \frac{1}{2}\nabla\mathrm{P}\boldsymbol{\eta} \cdot \mathbb{M}(\mathbf{q})\nabla\mathrm{P}\boldsymbol{\eta}\,\mathrm{d}x, \qquad \mathbb{M}(\boldsymbol{q}) = \frac{1}{e}\begin{pmatrix} n\mu_n & 0 \\ 0 & p\mu_p \end{pmatrix}, \tag{5}$$

where $\nabla\mathrm{P}\boldsymbol{\eta} \cdot \mathbb{M}\nabla\mathrm{P}\boldsymbol{\eta}$ means $\sum_i^d \partial_i(\mathrm{P}\boldsymbol{\eta})^\top\mathbb{M}\partial_i\mathrm{P}\boldsymbol{\eta}$. Here μ_n, $\mu_p > 0$ represent electron and hole mobilities. The dual dissipation potential comprising recombination and diffusion is given by $\Psi^*(\boldsymbol{q};\boldsymbol{\eta}) = \Psi_{\text{diff}}^*(\boldsymbol{q};\boldsymbol{\eta}) + \Psi_{\text{rec}}^*(\boldsymbol{q};\boldsymbol{\eta})$. Integrating by parts we find that the derivative of Ψ^* is

$$\langle \mathrm{D}_{\boldsymbol{\eta}}\Psi^*(\boldsymbol{q};\boldsymbol{\eta}), \boldsymbol{\nu}\rangle = \int_\Omega \boldsymbol{\nu}^\top\left[-\mathrm{P}^\top\nabla\cdot\mathbb{M}(\boldsymbol{q})\nabla\mathrm{P}\boldsymbol{\eta} + \mathbb{H}(\boldsymbol{q})\boldsymbol{\eta}\right]\mathrm{d}x \tag{6}$$

where $\boldsymbol{\nu} = (\nu_n, \nu_p, \nu_\gamma)$ with ν_n, ν_p are general functions and ν_γ is constant. When performing integration by parts we used appropriate boundary conditions for the boundary terms to vanish. By the properties of $\mathbb{M}$ we clearly see that $\mathrm{D}_{\boldsymbol{q}}\Psi^*(\boldsymbol{q};\cdot) : \boldsymbol{Q}\times\boldsymbol{Q}^* \to \mathbb{R}$ is a symmetric and positive semidefinite operator. Due to (3) we have

$$\partial_{\boldsymbol{c}}F(\boldsymbol{c},\theta_\star) = k_\mathrm{B}\theta_\star\begin{pmatrix}\log(n/\bar{n}) \\ \log(p/\bar{p}) \\ \log(\gamma/\bar{\gamma})\end{pmatrix} + \begin{pmatrix} E_\mathrm{c} - e\varphi_c \\ e\varphi_c - E_\mathrm{v} \\ 0\end{pmatrix}. \tag{7}$$

Then (6) and (7) lead to the abstract form

$$\dot{n} = -\nabla\cdot\boldsymbol{j}_n - \left[\Lambda_1(\partial_n F + \partial_p F) + (\Lambda_2 + \Lambda_3)(\partial_n F + \partial_p F - \partial_\gamma F)\right], \tag{8a}$$

$$\dot{p} = -\nabla\cdot\boldsymbol{j}_p - \left[\Lambda_1(\partial_n F + \partial_p F) + (\Lambda_2 + \Lambda_3)(\partial_n F + \partial_p F - \partial_\gamma F)\right], \tag{8b}$$

$$|\Omega|\dot{\gamma} = \int_\Omega (\Lambda_2 + \Lambda_3)\left[\partial_n F + \partial_p F - \partial_\gamma F\right]\mathrm{d}x, \tag{8c}$$

where the currents $\boldsymbol{j}_n$ and $\boldsymbol{j}_p$ are defined as

$$\begin{pmatrix} \boldsymbol{j}_n \\ \boldsymbol{j}_p \end{pmatrix} = -\mathbb{M}\nabla \begin{pmatrix} \partial_n F \\ \partial_p F \end{pmatrix} = -\mathbb{M}\nabla \begin{pmatrix} k_\mathrm{B}\theta_\star \log(n/\bar{n}) + E_\mathrm{c} - e\varphi_c \\ k_\mathrm{B}\theta_\star \log(p/\bar{p}) - E_\mathrm{v} + e\varphi_c \end{pmatrix}.$$

Using (4b) we get

$$\dot{n} = -\nabla\cdot \boldsymbol{j}_n - R_\mathrm{nr} - g(\boldsymbol{q})\left(\tfrac{np}{n_i^2} - \tfrac{\gamma}{\bar{\gamma}}\right), \tag{9a}$$

$$\dot{p} = -\nabla\cdot \boldsymbol{j}_p - R_\mathrm{nr} - g(\boldsymbol{q})\left(\tfrac{np}{n_i^2} - \tfrac{\gamma}{\bar{\gamma}}\right), \tag{9b}$$

$$|\Omega|\dot{\gamma} = -\left[\int_\Omega \frac{g(\boldsymbol{q})}{\bar{\gamma}}\,\mathrm{d}x\right]\gamma + \int_\Omega g(\boldsymbol{q})\frac{np}{n_i^2}\,\mathrm{d}x, \tag{9c}$$

where $\hat{n}\hat{p} = n_i^2(\theta_\star)$ and $\hat{\gamma} = \bar{\gamma}$. The term $R_\mathrm{nr} = k_1(\boldsymbol{q})(np/n_i^2 - 1)$, represents non-radiative recombination-generation processes. The rate of optical transitions $g(\boldsymbol{q}) = (\gamma/\bar{\gamma})k_2(\boldsymbol{q}) + k_3(\boldsymbol{q})$ includes stimulated and spontaneous absorption-emission and resembles optical gain in lasers. An equilibrium state of (9) is characterized by $n_\mathrm{eq}p_\mathrm{eq} = n_i^2$ and $\gamma_\mathrm{eq} = \bar{\gamma}$. To determine the equilibrium carrier densities $n_\mathrm{eq}, p_\mathrm{eq}$ requires to solve the Poisson equation (3d), which is nonlinear due to the insertion of $p_\mathrm{eq} = n_i\exp(-e\varphi_c/(k_\mathrm{B}\theta_\star))$ and $n_\mathrm{eq} = n_i\exp(e\varphi_c/(k_\mathrm{B}\theta_\star))$. With no-flux boundary conditions the gradient system (9) then implies a monotonous decay of the free energy towards this equilibrium

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{F}(\boldsymbol{c}(t)) = \langle \mathrm{D}_c\mathscr{F}, \dot{\boldsymbol{c}}\rangle = -\langle \mathrm{D}_c\mathscr{F}, \mathrm{D}_{\boldsymbol{\eta}}\Psi^*(\boldsymbol{c};\mathrm{D}_c\mathscr{F})\rangle \le 0 \tag{10}$$

as a consequence of the positive semi-definiteness of $\mathrm{D}_{\boldsymbol{\eta}}\Psi^*(\boldsymbol{q};\cdot)$.

Non-isothermal model. In the non-isothermal case it is advantegeous to start with the internal energy $u = U(\boldsymbol{c},\theta)$ as an independent variable, *cf.* [1]. Then, we solve (3b) for $\theta = \Theta(\boldsymbol{c},u)$ and set $\bar{\boldsymbol{q}} = (\boldsymbol{c},u) \in \boldsymbol{Q}$. We redefine energy and entropy as $\bar{\mathscr{U}}(\bar{\boldsymbol{q}}) = \int_\Omega u\,\mathrm{d}x$, and $\bar{\mathscr{S}}(\bar{\boldsymbol{q}}) = \mathscr{S}\big(\boldsymbol{c},\Theta(\boldsymbol{c},u)\big)$. For any functional $\Phi : \boldsymbol{Q} \to \mathbb{R}$ the derivative $\mathrm{D}_{\bar{\boldsymbol{q}}}\Phi(\bar{\boldsymbol{q}})$ now has four components. Therefore, the dual dissipation potential $\bar{\Psi}^*$ in the non-isothermal case can be obtained by extending the dual dissipation potential Ψ^* of the isothermal case as follows

$$\bar{\Psi}^*(\bar{\boldsymbol{q}};\boldsymbol{\eta}) = \int_\Omega \nabla(\mathrm{P}\boldsymbol{\eta})\cdot\bar{\mathbb{M}}(\bar{\boldsymbol{q}})\nabla\mathrm{P}\boldsymbol{\eta} + \boldsymbol{\eta}\cdot\bar{\mathbb{H}}(\bar{\boldsymbol{q}})\boldsymbol{\eta}\,\mathrm{d}x, \tag{11a}$$

$$\text{where}\qquad \bar{\mathbb{M}} = \Theta\begin{pmatrix} \mathbb{M} & \mathbb{M}_\mathrm{cross} \\ \mathbb{M}_\mathrm{cross}^\top & \mathbb{M}_u \end{pmatrix} \quad\text{and}\quad \bar{\mathbb{H}} = \Theta\begin{pmatrix} \mathbb{H} & 0 \\ 0 & 0 \end{pmatrix}, \tag{11b}$$

where $\mathrm{P} \in \mathbb{R}^{3\times 4}$ is a projector $\mathrm{P}\boldsymbol{\eta} = (\eta_n, \eta_p, \eta_u)$. Observe that $\mathrm{D}_{\bar{\boldsymbol{q}}}\bar{\mathscr{U}}(\boldsymbol{c},u) = (\boldsymbol{0},1)^\top$, so that the integrand in (11a) vanishes and thus also $\mathrm{D}_{\boldsymbol{\eta}}\bar{\Psi}^*(\bar{\boldsymbol{q}};\mathrm{D}_{\bar{\boldsymbol{q}}}\bar{\mathscr{U}}(\bar{\boldsymbol{q}})) = 0$. In turn, this implies the conservation of the internal energy $\bar{\mathscr{U}}(\bar{\boldsymbol{q}}(t))$ as

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\bar{\mathscr{U}} = \langle \mathrm{D}_{\bar{\boldsymbol{q}}}\bar{\mathscr{U}}, \dot{\bar{\boldsymbol{q}}}\rangle = \langle \mathrm{D}_{\bar{\boldsymbol{q}}}\bar{\mathscr{U}}, \mathrm{D}_{\boldsymbol{\eta}}\bar{\Psi}^*(\bar{\boldsymbol{q}};\mathrm{D}_{\bar{\boldsymbol{q}}}\bar{\mathscr{S}})\rangle = \langle \mathrm{D}_{\boldsymbol{\eta}}\bar{\Psi}^*(\bar{\boldsymbol{q}};\mathrm{D}_{\bar{\boldsymbol{q}}}\bar{\mathscr{U}}), \mathrm{D}_{\bar{\boldsymbol{q}}}\bar{\mathscr{S}}\rangle = 0,$$

where the last step follows from the symmetry of $\mathrm{D}_{\boldsymbol{\eta}}\bar{\Psi}^*(\bar{\boldsymbol{q}};\cdot)$. The evolution of the thermo-optoelectronic system is given by $\dot{\bar{\boldsymbol{q}}} = \mathrm{D}_{\boldsymbol{\eta}}\bar{\Psi}^*(\bar{\boldsymbol{q}};\mathrm{D}_{\bar{\boldsymbol{q}}}\bar{\mathscr{S}}(\bar{\boldsymbol{q}}))$ with the negative entropy as the driving functional. Since it is more common to write the equations using the temperature θ as a variable, we now reverse the previous change of variables and replace u with $U(\boldsymbol{c},\theta)$ and $\Theta(\boldsymbol{c},u)$ with θ and set $\Xi(\boldsymbol{c},\theta)=(\boldsymbol{c},U(\boldsymbol{c},\theta))$. This generates the transformed dual dissipation potential w.r.t. the variables $\boldsymbol{q}=(\boldsymbol{c},\theta)$ by $\Psi^*(\boldsymbol{c},\theta;\boldsymbol{\eta})=\bar{\Psi}^*(\Xi(\boldsymbol{c},\theta);A\boldsymbol{\eta})$ inducing $\dot{\boldsymbol{q}}=\mathrm{D}_{\boldsymbol{\eta}}\Psi^*(\boldsymbol{q};D_q\mathscr{S})$, where

$$A=\left(\mathrm{D}_{(c,\theta)}\Xi\right)^{-\top}=\begin{pmatrix}\mathbb{I}_{3\times 3} & -\frac{\partial_{\boldsymbol{c}}U}{\partial_\theta U}\\ 0 & \frac{1}{\partial_\theta U}\end{pmatrix},\qquad A(\boldsymbol{q})\partial_{\boldsymbol{q}}S(\boldsymbol{q})=\tfrac{1}{\theta}\begin{pmatrix}-\partial_{\boldsymbol{c}}F(\boldsymbol{c},\theta)\\ 1\end{pmatrix}.$$

The derivative $\mathrm{D}_{\boldsymbol{\eta}}\Psi^*$ is as in (6), but with a new projector P, we replaced $\boldsymbol{q}=\boldsymbol{c}$ by $\boldsymbol{q}=(\boldsymbol{c},\theta)$, $\boldsymbol{\eta}$ by $\mathrm{A}\boldsymbol{\eta}$, and $\mathbb{H},\mathbb{M}$ by $\bar{\mathbb{H}},\bar{\mathbb{M}}$. In addition to (8) but with temperature-dependent coefficients we obtain the following equation for the temperature

$$(\partial_\theta U)\dot{\theta}=-\nabla\cdot\boldsymbol{j}_\theta+(\partial_n U)(\nabla\cdot\boldsymbol{j}_n)+(\partial_p U)(\nabla\cdot\boldsymbol{j}_p)+(\partial_{\boldsymbol{c}}U)\cdot\mathbb{H}\partial_{\boldsymbol{c}}F,\tag{12}$$

with $(\partial_{\boldsymbol{c}}U)^\top=(-e\varphi_c+E_\mathrm{c},e\varphi_c-E_\mathrm{v},0)+\frac{1}{2}k_\mathrm{B}\theta(3,3,6)$ and the currents

$$\begin{pmatrix}\boldsymbol{j}_n\\ \boldsymbol{j}_p\\ \boldsymbol{j}_\theta\end{pmatrix}=\bar{\mathbb{M}}\nabla\frac{1}{\theta}\begin{pmatrix}\partial_n F\\ \partial_p F\\ -1\end{pmatrix}\equiv\bar{\mathbb{M}}\nabla\frac{1}{\theta}\begin{pmatrix}k_\mathrm{B}\theta\log(n/\bar{n})+E_\mathrm{c}-e\varphi_c\\ k_\mathrm{B}\theta\log(p/\bar{p})-E_\mathrm{v}+e\varphi_c\\ -1\end{pmatrix}.\tag{13}$$

Using $\Lambda_\mathrm{r}(\boldsymbol{c},\theta)$ from (4b) as in (9) we get the explicit form

$$\dot{n}=-\nabla\cdot\boldsymbol{j}_n-R_\mathrm{nr}-g(\boldsymbol{q})\left(\tfrac{np}{n_i^2}-\tfrac{\gamma}{\bar{\gamma}}\right),\tag{14a}$$

$$\dot{p}=-\nabla\cdot\boldsymbol{j}_p-R_\mathrm{nr}-g(\boldsymbol{q})\left(\tfrac{np}{n_i^2}-\tfrac{\gamma}{\bar{\gamma}}\right),\tag{14b}$$

$$|\Omega|\dot{\gamma}=-\left[\int_\Omega\frac{g(\boldsymbol{q})}{\bar{\gamma}}\,\mathrm{d}x\right]\gamma+\int_\Omega g(\boldsymbol{q})\frac{np}{n_i^2}\,\mathrm{d}x,\tag{14c}$$

$$\hat{c}_V\dot{\theta}=-\nabla\cdot\boldsymbol{j}_\theta+\sum_{i=1}^{2}\partial_{c_i}U(\nabla\cdot\boldsymbol{j}_{c_i})+\alpha_\mathrm{nr}R_\mathrm{nr}+\alpha_\mathrm{r}g\left(\tfrac{np}{n_i^2}-\tfrac{\gamma}{\bar{\gamma}}\right),\tag{14d}$$

where $\alpha_\mathrm{nr}=(\partial_n U+\partial_p U)=3k_\mathrm{B}\theta+E_\mathrm{g}$ and $\alpha_\mathrm{r}=(\partial_n U+\partial_p U+\partial_\gamma U)=6k_\mathrm{B}\theta+E_\mathrm{g}$, with the band gap is $E_\mathrm{g}=E_\mathrm{c}-E_\mathrm{v}$. The heat capacity $\hat{c}_V\equiv(\partial_\theta U)=c_V+k_\mathrm{B}\big(\frac{3}{2}(n+p)+3\gamma\big)+E_\mathrm{c}'(\theta)n-E_\mathrm{v}'(\theta)p$ is usually dominated by c_V. Note in general $E_\mathrm{c},E_\mathrm{v},\bar{n},\bar{p}$ depends on space and temperature, which will then consistently generate extra drift terms in the current in (13). Also observe that the same calculations as in (10) with $\mathrm{D}\mathscr{S}$ instead of $-\mathrm{D}\mathscr{F}$ provide the production of entropy $\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{S}(\boldsymbol{q}(t))\geq 0$.

3 Discussion

The non-isothermal model derived here is in the spirit of [2], but our approach is focussed on a concise derivation in the framework of gradient structures. Since a term-by-term comparison is beyond the scope of this paper let us mention a few key differences. The model in [2] is for a semiconductor laser, for which additionally light is spatially localized in a mode density χ solving a Helmholtz equation. Even though one can easily modify the functionals to create similar looking terms, *e.g.*, g is replaced by $g|\chi|^2$ in the emission-absorption, the coherent, and in this sense more luminescent, character of light makes a thermodynamic approach using entropies more elusive. We believe that using the GENERIC formalism to couple the charge transport to Hamiltonian system which are either more microscopic, *e.g.*, quantum mechanical [9], or to the classical Maxwell equation might help to clarify the situation. For the shortness of the presentation we assumed homogeneous natural boundary conditions of vanishing normal fluxes and obtained the decay of the free energy. Obviously the model is built so that it also supports electrical pumping of a photon field, *i.e.*, an energy flux through non-homogeneous boundary conditions.

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