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On thermodynamical couplings of quantum mechanics and macroscopic systems

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Abstract

Pure quantum mechanics can be formulated as a Hamiltonian system in terms of the Liouville equation for the density matrix. Dissipative effects are modeled via coupling to a macroscopic system, where the coupling operators act via commutators. Following Öttinger (2010) we use the GENERIC framework to construct thermodynamically consistent evolution equations as a sum of a Hamiltonian and a gradient-flow contribution, which satisfy a particular non-interaction condition:

$$\dot{q} = \mathbb{J}(q)\mathrm{D}\mathcal{E}(q) + \mathbb{K}(q)\mathrm{D}\mathcal{S}(q).$$

We give three applications of the theory. First, we consider a finite-dimensional quantum system that is coupled to a finite number of simple heat baths, each of which is described by a scalar temperature variable. Second, we model quantum system given by a one-dimensional Schrödinger operator connected to a one-dimensional heat equation on the left and on the right. Finally, we consider thermo-opto-electronics, where the Maxwell-Bloch system of optics is coupled to the energy-drift-diffusion system for semiconductor electronics.

1 Introduction

A fundamental problem in nano-science is a consistent coupling of quantum mechanics with effects on larger scales, see [KW*11] for the modeling of lasers based on quantum-dot layers. In particular, one is interested in combining quantum and continuum mechanical models with dissipative effects in such a way that the fundamental axioms of thermodynamics and quantum mechanics are still satisfied. We follow [Ött10, Ött11] in modeling the coupling between classical dissipative systems and reversible quantum systems formulated in terms of the Liouville equation for the density matrix. The basis is the theory of GENERIC systems, which stands for the acronym General Equations for Non-Equilibrium Reversible Irreversible Coupling and which was developed earlier under the name metriplectic system, see [Mor86] and [BMR13, Sect. 15.4] for the history.

A GENERIC system is a quintuple $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$ with state space $\mathcal{Q}$, total energy $\mathcal{E} : \mathcal{Q} \to \mathbb{R}$ and total entropy $\mathcal{S} : \mathcal{Q} \to \mathbb{R}$. The evolution equation reads

$$\dot{q} = \mathbb{J}(q)\mathrm{D}\mathcal{E}(q) + \mathbb{K}(q)\mathrm{D}\mathcal{S}(q), \tag{1.1}$$

which displays an additive split into a Hamiltonian part $\mathbb{J}(q)\mathrm{D}\mathcal{E}(q)$, where $\mathbb{J}$ is a Poisson structure, and a dissipative part $\mathbb{K}(q)\mathrm{D}\mathcal{S}(q)$, where the Onsager operator $\mathbb{K}$ satisfies $\mathbb{K} = \mathbb{K}^* \geq 0$. GENERIC systems are thermodynamically correct in the sense that the total energy $\mathcal{E}$ is preserved while the total entropy $\mathcal{S}$ is nondecreasing. This is guaranteed by the central non-interaction conditions

$$\textbf{(NIC)} \qquad \mathbb{J}(q)\mathrm{D}\mathcal{S}(q) \equiv 0 \quad \text{and} \quad \mathbb{K}(q)\mathrm{D}\mathcal{E}(q) \equiv 0. \tag{1.2}$$

The evolution of the quantum mechanical system on a Hilbert space $\boldsymbol{H}$ will be described in terms of the density matrix $\rho \in \mathfrak{R} := \{\, \rho \in \mathcal{L}^1(\boldsymbol{H}) \mid 0 \leq \rho = \rho^*,\ \operatorname{tr}\rho = 1 \,\}$ and the Liouville equation $\dot{\rho} = \frac{\mathrm{i}}{\hbar}[\rho, H]$, where $H = H^*$ is the Hamiltonian. Following [Ött10, Ött11] we couple this quantum system to the dissipative system $\dot{z} = \mathbb{K}_{\mathrm{di}}(z)\mathrm{D}\mathcal{S}_{\mathrm{di}}(z)$

using observables $Q_m = Q_m^*$ as coupling operators. In Section 2.4 we show that

$$\begin{aligned} \dot\rho &= \jmath\big[\rho, H\big] - \sum_{m=1}^{M} \Big(\big[\, Q_m \,,\, k_\mathrm{B}[Q_m,\rho] + \mathcal{C}_\rho[Q_m, \mathrm{B}_m(z)\mathrm{D}\mathcal{S}_\mathrm{di}(z)]\,\big] \Big), \\ \dot z &= \qquad\quad \mathbb{K}_\mathrm{di}(z)\mathrm{D}\mathcal{S}_\mathrm{di}(z) + \sum_{m=1}^{M} \mathrm{B}_m^*(z) \big[\, Q_m \,,\, k_\mathrm{B}[Q_m,\rho] + \mathcal{C}_\rho[Q_m, \mathrm{B}_m(z)\mathrm{D}\mathcal{S}_\mathrm{di}(z)]\,\big] \end{aligned} \tag{1.3}$$

with $\mathbb{K}_\mathrm{di}\mathrm{D}\mathcal{E}_\mathrm{di} \equiv 0$ and $\mathrm{B}_m\mathrm{D}\mathcal{E}_\mathrm{di} \equiv H$ for $m = 1, ..., M$ is a GENERIC system for

$$\mathcal{E}(\rho, z) = \mathrm{tr}(\rho H) + \mathcal{E}_\mathrm{di}(z) \quad \text{and} \quad \mathcal{S}(\rho, z) = -k_\mathrm{B}\, \mathrm{tr}(\rho \log \rho) + \mathcal{S}_\mathrm{di}(z).$$

The crucial mathematical structure in our theory of the so-called canonical correlation operator $\mathcal{C}_\rho : \mathcal{L}^\infty(\boldsymbol{H}) \to \mathcal{L}^1(\boldsymbol{H})$ given by

$$\mathcal{C}_\rho A := \int_0^1 \rho^s A \rho^{1-s}\, \mathrm{d}s \quad \text{and} \quad \mathcal{C}_\rho^{-1} B = \int_0^\infty (\rho{+}sI)^{-1} B (\rho{+}sI)^{-1}\, \mathrm{d}s,$$

see [Gra82, Ött10, Ött11] for its justification via fluctuation theory. The inverse $\mathcal{C}_\rho^{-1}$ is called the Bogoliubov-Kubo-Mori metric, cf. [Str96, MPA00]. There is a strong relation between the von Neumann entropy and $\mathcal{C}_\rho$ encoded in the fundamental commutator relations

$$\big[\mathcal{C}_\rho A, \log \rho\big] = \big[A, \rho\big] = \mathcal{C}_\rho\big[A, \log\rho\big], \tag{1.4}$$

for all $A = A^*$ and $\rho \in \mathfrak{R}$. Recall $\mathrm{D}_\rho \mathcal{S} = -k_\mathrm{B} \log \rho$ and note that $\mathrm{D}_\rho^2 \mathcal{S} = \mathcal{C}_\rho^{-1}$, see [MPA00, CaM12]. The continuity of $\rho \mapsto \mathcal{C}_\rho$ is proved in [Mie13, Prop. 21.2], see (2.18).

In Section 2 we give the basic features of GENERIC system, introduce the relevant notation for quantum systems, and describe the general principles of coupling in terms of commutators $[Q_m, \cdot\,]$ with coupling operators and the canonical correlation operator. In Section 3 we consider the finite-dimensional model that is obtained by assuming $\dim \boldsymbol{H} < \infty$ and $z = (\theta_1, ..., \theta_M) \in\,]0, \infty[^M$. We give a short overview of the results of [Mie13].

In Section 4 we discuss a quantum dot described by a one-dimensional Schrödinger operator that is coupled to a left and a right reservoir described by a heat equation. Here we also address the question of the existence of non-equilibrium steady states, which arises if the specific heat of the reservoirs tends to infinity. We also conjecture suitable formulas for the flux through the quantum dot if the temperature of the two reservoirs is different.

Section 5 is devoted to thermo-opto-electronics, which couples the Maxwell-Bloch system for optics in a crystal with polarization to the semiconductor equations for temperature and drift-diffusion for the charge carriers. The former is a Hamiltonian system (cf. [JMR00, Dum05]), while the latter was shown to be a gradient system in [Mie11b]. See [BKM14] for the full details.

2 Coupling of quantum and dissipative mechanics

We first introduce the notion of GENERIC systems and then specify to the case where the underlying Hamiltonian system is given by a quantum mechanical system. In Section 2.4 we introduce the Kubo-Mori metric on density matrices, which provides a canonical way of defining dissipation in quantum systems.

2.1 The GENERIC framework

The framework of GENERIC was introduced by Morrison [Mor86] under the name *metriplectic systems*, see [BMR13, Sec. 15.4] for an outline of these early developments. In [GrÖ97, ÖtG97] Öttinger and Grmela introduced the name GENERIC to emphasize the thermodynamical modeling aspects that were relevant for their applications in fluid mechanics. A more mathematical formulation is given in [Mie11a], where applications to thermoplasticity are developed. A survey on the modeling aspects of GENERIC and various applications will be presented in [MiT14]. Our subsequent discussion is mainly based on the quantum mechanical papers [Ött10, Ött11].

A GENERIC system is a quintuple $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$, where the smooth functionals $\mathcal{E}$ and $\mathcal{S}$ on the state space $\mathcal{Q}$ denote the total energy and the total entropy, respectively. Moreover, $\mathcal{Q}$ carries two geometric structures, namely a Poisson structure $\mathbb{J}$ and a dissipative Onsager structure $\mathbb{K}$, i.e., for each $q \in \mathcal{Q}$ the operators $\mathbb{J}(q)$ and $\mathbb{K}(q)$ map the cotangent space $\mathrm{T}_q^*\mathcal{Q}$ into the tangent space $\mathrm{T}_q\mathcal{Q}$. The evolution of the system is given as the sum of the Hamiltonian part $\mathbb{J}(q)\mathrm{D}\mathcal{E}(q)$ and the gradient-flow $\mathbb{K}(q)\mathrm{D}\mathcal{S}(q)$, namely

$$\dot{q} = \mathbb{J}(q)\mathrm{D}\mathcal{E}(q) + \mathbb{K}(q)\mathrm{D}\mathcal{S}(q). \tag{2.1}$$

The basic conditions on the geometric structures $\mathbb{J}$ and $\mathbb{K}$ are the symmetries

$$\mathbb{J}(q) = -\mathbb{J}(q)^* \text{ and } \mathbb{K}(q) = \mathbb{K}(q)^* \tag{2.2}$$

and the structural properties

$$\begin{aligned}&\mathbb{J} \text{ satisfies Jacobi's identity,}\\ &\mathbb{K}(q) \text{ is positive semi-definite, i.e., } \langle \xi, \mathbb{K}(q)\xi\rangle \geq 0.\end{aligned} \tag{2.3}$$

Here, Jacobi's identity for $\mathbb{J}$ holds, if

$$\langle \eta_1, \mathrm{D}\mathbb{J}(q)[\mathbb{J}(q)\eta_2]\eta_3\rangle + \langle \eta_2, \mathrm{D}\mathbb{J}(q)[\mathbb{J}(q)\eta_3]\eta_1\rangle + \langle \eta_3, \mathrm{D}\mathbb{J}(q)[\mathbb{J}(q)\eta_1]\eta_2\rangle = 0 \text{ for all } \eta_j \in \mathrm{T}_q^*\mathcal{Q}.$$

The central condition states that the energy functional does not contribute to dissipative mechanisms and that the entropy functional does not contribute to reversible dynamics, which is the following *non-interaction condition*:

$$\textbf{(NIC)} \qquad \forall\, q \in \mathcal{Q}: \quad \mathbb{J}(q)\mathrm{D}\mathcal{S}(q) = 0 \quad \text{and} \quad \mathbb{K}(q)\mathrm{D}\mathcal{E}(q) = 0. \tag{2.4}$$

Of course, the structure of GENERIC is geometric in the sense that it is invariant under coordinate transformations, see [Mie11a, MiT14]. The first observation is that (2.3) and (2.4) imply energy conservation and entropy increase:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(q(t)) = \langle \mathrm{D}\mathcal{E}(q), \dot{q}\rangle = \langle \mathrm{D}\mathcal{E}(q), \mathbb{J}\mathrm{D}\mathcal{E} + \mathbb{K}\mathrm{D}\mathcal{S}\rangle = 0 + 0 = 0, \tag{2.5}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(q(t)) = \langle \mathrm{D}\mathcal{S}(q), \dot{q}\rangle = \langle \mathrm{D}\mathcal{S}(q), \mathbb{J}\mathrm{D}\mathcal{E} + \mathbb{K}\mathrm{D}\mathcal{S}\rangle = 0 + \langle \mathrm{D}\mathcal{S}, \mathbb{K}\mathrm{D}\mathcal{S}\rangle \geq 0. \tag{2.6}$$

Of course, to guarantee energy conservation and positivity of the entropy production one needs much less than the two conditions (2.3) and (2.4).

However, the *maximum entropy principle* really relies on (2.4). It states that a maximizer q_* of $\mathcal{S}$ subject to the constraint $\mathcal{E}(q) = E_0$ is an equilibrium of (2.1), the so-called thermodynamic equilibrium for the given energy. Indeed, if q_* maximizes $\mathcal{S}$ under the constraint $\mathcal{E}(q) = E_0$, then we obtain a Lagrange multiplier $\lambda_{\mathsf{eq}} \in \mathbb{R}$ such that $\mathrm{D}\mathcal{S}(q_*) = \lambda_* \mathrm{D}\mathcal{E}(q_*)$. Since $\mathrm{D}\mathcal{S}(q) \neq 0$ for all q (e.g. by $\partial_\theta S > 0$), we have $\lambda_* \neq 0$ and conclude $\mathbb{J}(q_*)\mathrm{D}\mathcal{E}(q_*) = \frac{1}{\lambda_{\mathsf{eq}}}\mathbb{J}(q_*)\mathrm{D}\mathcal{S}(q_*) = 0$ and $\mathbb{K}(q_*)\mathrm{D}\mathcal{S}(q_*) = \lambda_{\mathsf{eq}}\mathbb{K}(q_*)\mathrm{D}\mathcal{E}(q_*) = 0$, where we have used the NIC (2.4). Vice versa, every steady state q_* of (2.1) satisfies

$$\mathbb{J}(q_*)\mathrm{D}\mathcal{E}(q_*) = 0 \text{ and } \mathbb{K}(q_*)\mathrm{D}\mathcal{S}(q_*) = 0. \tag{2.7}$$

Thus, in a steady state there cannot be any balancing between reversible and irreversible forces, both have to vanish independently.

To show (2.7) we simply recall the entropy production relation (2.6), which implies $\langle \mathrm{D}\mathcal{S}(q_*), \mathbb{K}(q_*)\mathrm{D}\mathcal{S}(q_*)\rangle = 0$ for any steady state. Since $\mathbb{K}(q_*)$ is positive semidefinite, this implies the second identity in (2.7). The first identity then follows from $\dot{q} \equiv 0$ in (2.1).

2.2 Quantum mechanics

The quantum mechanical system is described by states in a complex Hilbert space $\boldsymbol{H}$ with scalar product $\langle \cdot | \cdot \rangle$ and a Hamiltonian (operator) $H : D(H) \to \boldsymbol{H}$, which is assumed to be selfadjoint and semi-bounded, namely

$$\exists\, h_{\min} \in \mathbb{R}\ \forall \psi \in D(H): \quad \langle H\psi|\psi\rangle \geq h_{\min}\|\psi\|^2.$$

The associated Hamiltonian dynamics is given via the time-dependent Schrödinger equation $\dot{\psi} = -\jmath H\psi$, where $\jmath = \frac{\mathrm{i}}{\hbar}$, which has the solution $\psi(t) = \mathrm{e}^{-\jmath t H}\psi(0)$.

We denote by $\mathcal{L}^p(\boldsymbol{H})$ the Banach space of compact operators A from $\boldsymbol{H}$ into itself with norm $\|A\|_p := \big(\sum_{j=1}^\infty \sigma_j(A)^p\big)^{1/p}$, where σ_j is the jth singular value of A, see [GoK69, Ch. III]. Moreover, $\mathcal{L}^\infty(\boldsymbol{H})$ is the set of bounded linear operators. On $\mathcal{L}^1(\boldsymbol{H})$ the trace operator $\mathrm{tr} : \mathcal{L}^1(\boldsymbol{H}) \to \mathbb{C},\ A \mapsto \sum_{j=1}^\infty \langle A\phi_j|\phi_j\rangle$ is well-defined, where $\{\, \phi_j \mid j \in \mathbb{N}\,\}$ is an arbitrary complete orthonormal system in $\boldsymbol{H}$. Using the dual pairing

$$\langle\!\langle\, A \,\|\, B \,\rangle\!\rangle := \mathrm{tr}(AB^*), \text{ where } \mathrm{tr}(\psi \otimes \overline{\phi}) = \langle \psi|\phi\rangle,$$

we see that $\mathcal{L}^2(\boldsymbol{H})$ is a Hilbert space. By $\mathcal{L}^p_{\mathrm{S}}(\boldsymbol{H})$ we denote the subspace of symmetric bounded linear operators in $\mathcal{L}^p(\boldsymbol{H})$. The coupling of a quantum system to a macroscopic one can be described using the density matrices

$$\rho \in \mathfrak{R} := \{\, \rho \in \mathcal{L}^1(\boldsymbol{H}) \mid \rho = \rho^* \geq 0,\ \mathrm{tr}\,\rho = 1 \,\} \ \subset\ \mathcal{L}^1_{\mathrm{S}}(\boldsymbol{H}).$$

Each $\rho \in \mathfrak{R}$ has the representation $\rho = \sum_{j=1}^\infty r_j\, \psi_j \otimes \overline{\psi}_j$, where $r_j \geq 0$, $\sum_1^\infty r_j = 1$, and $\{\, \psi_j \mid j \in \mathbb{N}\,\}$ is an orthonormal set. The evolution of ρ is given via the Liouville equation

$$\dot{\rho} = \jmath[\rho, H], \quad \text{where } [\rho, H] := \rho H - H\rho. \tag{2.8}$$

Below we will use the *von Neumann entropy*

$$\mathcal{S}_{\mathrm{qm}}(\rho) = -k_{\mathrm{B}}\langle\!\langle\, \rho \,\|\, \log\rho \,\rangle\!\rangle = -k_{\mathrm{B}}\,\mathrm{tr}(\rho\log\rho) = -k_{\mathrm{B}}\textstyle\sum_{j=1}^\infty r_j \log r_j, \tag{2.9}$$

which remains constant along the solutions ρ of the Hamiltonian system (2.8).

Defining $\mathcal{Q} = \mathfrak{R}$, $\mathcal{E}_{\mathrm{qm}}(\rho) = \mathrm{tr}(\rho H)$, $\mathbb{J}_{\mathrm{qm}}(\rho) = \jmath[\rho, \Box]$ (where "$\Box$" indicates the place to insert the argument), and $\mathbb{K}_{\mathrm{qm}} \equiv 0$, we see that (2.8) is given by the purely Hamiltonian GENERIC system $(\mathfrak{R}, \mathcal{E}_{\mathrm{qm}}, \mathcal{S}_{\mathrm{qm}}, \mathbb{J}_{\mathrm{qm}}, 0)$.

2.3 General coupling of QM to dissipative models

We consider an additional variable $z \in \mathcal{Z}$ which is driven by a a gradient flow

$$\dot{z} = \mathbb{K}_{\mathrm{di}}(z)\mathrm{D}\mathcal{S}_{\mathrm{di}}(z), \text{ where } \mathbb{K}_{\mathrm{di}}(z) = \mathbb{K}_{\mathrm{di}}(z)^* \geq 0. \tag{2.10}$$

We call such systems *Onsager systems*, because of Onsager's fundamental contributions in [Ons31, Part II, (1.11)], where the symmetry $\mathbb{K}_{\mathrm{di}}(z) = \mathbb{K}_{\mathrm{di}}(z)^*$ was derived, see also [OnM53, eqns. (2-1) to (2-4)], where it is stated that (2.10) is the universal form for many physical systems close to (local) equilibrium such as Ohm's law, Fick's law, heat flow, etc. We assume that (2.10) preserves an energy $\mathcal{E}_{\mathrm{di}}$ via the condition $\mathbb{K}_{\mathrm{di}}(z)\mathrm{D}\mathcal{E}_{\mathrm{di}}(z) \equiv 0$.

Following [Ött10, Ött11] we couple the above quantum system to the Onsager system in the GENERIC framework by setting $\mathcal{Q} = \mathfrak{R} \times \mathcal{Z}$ and using an additive split of the energy and the entropy:

$$\mathcal{E}(\rho, z) = \langle\!\langle\, H(z) \,\|\, \rho \,\rangle\!\rangle + \mathcal{E}_{\mathrm{di}}(z) \quad \text{and} \quad \mathcal{S}(\rho, z) = -k_{\mathrm{B}}\langle\!\langle\, \rho \,\|\, \log \rho \,\rangle\!\rangle + \mathcal{S}_{\mathrm{di}}(z).$$

In the general case, the Hamiltonian H may depend on the dissipative variable z (see e.g. (5.1) and (5.3)), but for the moment we assume that H is independent of z. We obtain the thermodynamic driving forces

$$\begin{pmatrix} \widetilde{\mu} \\ \widetilde{\zeta} \end{pmatrix} = \mathrm{D}\mathcal{E}(\rho, z) = \begin{pmatrix} H \\ \mathrm{D}_z\mathcal{E}_{\mathrm{di}}(z) \end{pmatrix}, \quad \begin{pmatrix} \mu \\ \zeta \end{pmatrix} = \mathrm{D}\mathcal{S}(\rho, z) = \begin{pmatrix} \mathrm{D}_\rho\mathcal{S}_{\mathrm{qm}}(\rho) \\ \mathrm{D}_z\mathcal{S}_{\mathrm{di}}(z) \end{pmatrix} = \begin{pmatrix} -k_{\mathrm{B}} \log \rho \\ \mathrm{D}\mathcal{S}_{\mathrm{di}}(z) \end{pmatrix}.$$

Since z is a totally dissipative variable, the coupled Poisson structure $\mathbb{J}$ reads

$$\mathbb{J}(\rho, z) = \begin{pmatrix} \mathbb{J}_{\mathrm{qm}}(\rho) & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} \jmath[\rho, \Box\,] & 0 \\ 0 & 0 \end{pmatrix}, \tag{2.11}$$

and using $[\rho, \log \rho] \equiv 0$ we see that $(\mathrm{NIC})_1$ (i.e. $\mathbb{J}\mathrm{D}\mathcal{S} \equiv 0$) is satisfied.

The Onsager operator $\mathbb{K}$ of the coupled system is the sum of $\mathbb{K}_{\mathrm{di}}$ and a dissipative coupling between the variables ρ and z. We will write it in terms of the dual entropy-production potential $\mathcal{R}^*(\rho, z, \mu, \zeta) = \frac{1}{2}\langle\binom{\mu}{\zeta}, \mathbb{K}(\rho, z)\binom{\mu}{\zeta}\rangle$. Using $\mathbb{K} \geq 0$ it is easy to see

$$(\mathrm{NIC})_2 \quad \Longleftrightarrow \quad \mathcal{R}^*(\rho, z, \mathrm{D}\mathcal{E}(\rho, z)) = \mathcal{R}^*(\rho, z, H, \mathrm{D}\mathcal{E}_{\mathrm{di}}(z)) \equiv 0.$$

As in [Ött10, Ött11] we assume that the quantum system can only couple to the dissipative macroscopic system via observables, which are given by commutators with symmetric bounded linear operators $Q(z) \in \mathcal{L}^\infty_{\mathrm{S}}(\boldsymbol{H})$. Hence, a possible form for $\mathcal{R}^*$ is

$$\mathcal{R}^*(\rho, z, \mu, \zeta) = \frac{1}{2}\langle \zeta, \mathbb{K}_{\mathrm{di}}(z)\zeta\rangle + \frac{1}{2}\sum_{m=1}^{M} \big|\!\big|\!\big| [Q_m(z), \mu - \mathrm{B}_m(z)\zeta] \big|\!\big|\!\big|^2_{\mathfrak{C}_m(\rho, z)},$$

where $\mathrm{B}_m(z)$ is a linear operator from $\mathrm{T}^*_z\mathcal{Z}$ to self-adjoint operators on $\boldsymbol{H}$ such that $\mathrm{B}_m(z)\mathrm{D}\mathcal{E}_{\mathrm{di}}(z) \equiv H$. The norms $|\!|\!|\cdot|\!|\!|_{\mathfrak{C}}$ are given via

$$|\!|\!| A |\!|\!|_{\mathfrak{C}} := \langle\!\langle\, \mathfrak{C}A \,\|\, A \,\rangle\!\rangle^{1/2} = \|\mathfrak{C}^{1/2}A\|_2,$$

where the super-operators $\mathfrak{C}_m(\rho, z)$ is symmetric and positive semidefinite on $\mathcal{L}^2(\boldsymbol{H})$ (where super-operators are linear operator on $\mathcal{L}^p(\boldsymbol{H})$). Using the notation $\mathfrak{K}^Q_{\mathfrak{C}}A := [Q^*, \mathfrak{C}[Q, A]]$ we can write the Onsager operator $\mathbb{K}$ in the form

$$\mathbb{K}(q) = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{K}_{\mathrm{di}}(z) \end{pmatrix} + \sum_{m=1}^{M} \begin{pmatrix} \mathfrak{K}^{Q_m}_{\mathfrak{C}_m} & -\mathfrak{K}^{Q_m}_{\mathfrak{C}_m}\mathrm{B}_m(z) \\ -\mathrm{B}^*_m(z)\mathfrak{K}^{Q_m}_{\mathfrak{C}_m} & \mathrm{B}^*_m(z)\mathfrak{K}^{Q_m}_{\mathfrak{C}_m}\mathrm{B}_m(z) \end{pmatrix}. \tag{2.12}$$

The above assumptions guarantee that $(\mathfrak{R}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$ provides a GENERIC system. The evolution equations for $q = (\rho, z)$ are the coupled system

$$\begin{aligned} \dot\rho &= \jmath[\rho, H] - \sum_{m=1}^{M} \mathbb{K}^{Q_m(z)}_{\mathfrak{C}_m(\rho,z)}\Big(k_\mathrm{B}\log\rho + \mathrm{B}_m(z)\mathrm{D}\mathcal{S}_\mathrm{di}(z)\Big),\\ \dot z &= \qquad \mathbb{K}_\mathrm{di}(z)\mathrm{D}\mathcal{S}_\mathrm{di}(z) + \sum_{m=1}^{M} \mathrm{B}^*_m(z)\,\mathbb{K}^{Q_m(z)}_{\mathfrak{C}_m(\rho,z)}\Big(k_\mathrm{B}\log\rho + \mathrm{B}_m(z)\mathrm{D}\mathcal{S}_\mathrm{di}(z)\Big). \end{aligned} \tag{2.13}$$

2.4 The Kubo-Mori metric

In [Gra82, Ött11, Mie13] it is argued that the dissipative super-operators $\mathfrak{C}_m$ should be given by the *canonical correlation operator* $\mathcal{C}_\rho$, which associates with the density matrix $\rho \in \mathfrak{R}$ in the following way:

$$\mathcal{C}_\rho : \left\{ \begin{array}{ccc} \mathcal{L}^\infty(\boldsymbol{H}) & \to & \mathcal{L}^1(\boldsymbol{H}), \\ A & \mapsto & \int_0^1 \rho^s A \rho^{1-s}\,\mathrm{d}s. \end{array} \right. \tag{2.14}$$

By $\rho = \rho^*$ one has $(\mathcal{C}_\rho A)^* = \mathcal{C}_\rho(A^*)$, and if $\rho = \sum r_j \psi_j \otimes \overline{\psi}_j$, then

$$\mathcal{C}_\rho A = \sum_{j,k=1}^{\dim \boldsymbol{H}} \Lambda(r_j, r_k)\langle A\psi_k|\psi_j\rangle \psi_j \otimes \overline{\psi}_k \text{ and } \langle\!\langle\, \mathcal{C}_\rho A \,\|\, A \,\rangle\!\rangle = \sum_{j,k=1}^{\dim \boldsymbol{H}} \Lambda(r_j, r_k)\big|\langle A\psi_k|\psi_j\rangle\big|^2 \tag{2.15}$$

with $\Lambda(a, b) = \int_0^1 a^s b^{1-s}\,\mathrm{d}s$. In particular, $\mathcal{C}_\rho$ is symmetric and positive semidefinite:

$$\langle\!\langle\, \mathcal{C}_\rho A \,\|\, B \,\rangle\!\rangle = \langle\!\langle\, A \,\|\, \mathcal{C}_\rho B \,\rangle\!\rangle \quad \text{and} \quad \langle\!\langle\, \mathcal{C}_\rho A \,\|\, A \,\rangle\!\rangle \geq 0.$$

Hence, $\mathcal{C}_\rho$ induces the scalar product $\langle A, B\rangle_\rho := \langle\!\langle\, \mathcal{C}_\rho A \,\|\, B \,\rangle\!\rangle$, which is called the *canonical correlation between A and B for the given state ρ* in [KTH91, Ött11].

For $\rho > 0$ and $\dim \boldsymbol{H} < \infty$ the operator $\mathcal{C}_\rho$ is invertible, namely

$$\mathcal{G}_\rho A := \mathcal{C}_\rho^{-1} A = \int_0^\infty (\rho + sI)^{-1} A (\rho + sI)^{-1}\,\mathrm{d}s, \tag{2.16}$$

which can be derived from (2.15) using $1/\Lambda(a, b) = \int_0^\infty \big((a+s)(b+s)\big)^{-1}\,\mathrm{d}s$. The super-operator $\mathcal{G}_\rho$ defines the *Bogoliubov-Kubo-Mori metric* on the set of density matrices as follows, see [Pet94, MPA00].

For us, the most important fact is the connection to the von Neumann entropy $\mathcal{S}_\mathrm{qm}$, see (2.9). In fact, $\mathcal{G}_\rho$ can be identified by its Hessian up to the factor $-k_\mathrm{B}$, namely $\langle\!\langle\, A \,\|\, \mathrm{D}^2 S_\mathrm{qm}(\rho) B \,\rangle\!\rangle = -k_\mathrm{B} \langle\!\langle\, A \,\|\, \mathcal{G}_\rho B \,\rangle\!\rangle$. In particular, we will heavily use the identities

$$\big[\mathcal{C}_\rho A, \log\rho\big] = \big[A, \rho\big] = \mathcal{C}_\rho\big[A, \log\rho\big], \tag{2.17}$$

which go back to [Kub66], play an important role in the field of dissipative effects in quantum mechanics and manifest the relation between the von Neumann entropy $\mathcal{S}_\mathrm{qm}$ and the canonical correlation operator $\mathcal{C}_\rho$. See [Mie13, Prop. 21.1] for a simple proof and [CaM12, Lem. 3.1], where a general calculus for operator functions is developed. (These identities generalize the differential identity $v\nabla(\log v) = \nabla v$, which is crucial for the entropic gradient formulation of the Fokker-Planck equation, see [Ott01] and [Mie13, Sect. 21.7] for a comparison of the different gradient structures.)

In addition, [Mie13, Prop. 21.2] provides the continuity of $\mathcal{C}_\rho$ in the form

$$\|\mathcal{C}_{\rho_1}A-\mathcal{C}_{\rho_2}A\|_1 \leq \omega\Big(\tfrac{\|\rho_1-\rho_2\|_1}{\|\rho_1\|_1+\|\rho_2\|_1}\Big)\big(\|\rho_1\|_1+\|\rho_2\|_1\big)\|A\|_\infty, \quad \omega(\nu)=2\tfrac{1-\nu}{|\log\nu|}. \tag{2.18}$$

We emphasize that $\mathfrak{R} \ni \rho \mapsto \mathcal{C}_\rho \in \mathrm{Lin}(\mathcal{L}^\infty_{\mathrm{S}}(\boldsymbol{H}), \mathcal{L}^1_{\mathrm{S}}(\boldsymbol{H})$ is continuous, if $\mathfrak{R}$ is equipped with the norm of $\mathcal{L}^1_{\mathrm{S}}(\boldsymbol{H})$.

If we specialize the general coupled system (2.13) by choosing all $\mathfrak{C}_m$ equal to $\mathcal{C}_\rho$, as suggested in [Ött11], we can use the identities (2.17) which yields $\mathfrak{K}^Q_{\mathcal{C}_\rho}\log\rho = \big[Q,[Q,\rho]\big]$, where the right-hand side is continuous. Thus, the singularity in $\log\rho$ and the nonlinearity of $\mathcal{C}_\rho$ interact in a nice way to give rise to a linear and hence continuous term. Hence, (2.13) takes the form (where we dropped the dependence of Q_m on z for simplicity):

$$\begin{aligned} \dot\rho &= \jmath\big[\rho,H\big] - \sum_{m=1}^M \Big(\big[\,Q_m\,,\,k_\mathrm{B}[Q_m,\rho] + \mathcal{C}_\rho[Q_m,G_m(z)]\,\big]\Big),\\ \dot z &= \qquad\quad \mathbb{K}_\mathrm{di}(z)\mathrm{D}\mathcal{S}_\mathrm{di}(z) + \sum_{m=1}^M \mathrm{B}^*_m(z)\big[\,Q_m\,,\,k_\mathrm{B}[Q_m,\rho] + \mathcal{C}_\rho[Q_m,G_m(z)]\,\big], \end{aligned} \tag{2.19}$$

where $G_m(z) := \mathrm{B}_m(z)\mathrm{D}\mathcal{S}_\mathrm{di}(z)$. We see the analogy to the so-called Lindblad equations

$$\dot\rho = \jmath[\rho,H] - k_\mathrm{B}\sum_{m=1}^M \big[Q_m,[Q_m,\rho]\big],$$

where the double bracket terms generate the dissipation, see e.g. [Gra82, Lin76, Arn08].

The most important feature of this system is that the singular term $\log\rho$ in the right-hand side has disappeared. Under suitable further assumptions the right-hand side forms a continuous vector field, which wasn't the case for (2.13).

3 A finite-dimensional model with simple heat baths

In this section we consider a finite-dimensional version of the general coupled system developed above. We will summarize the results obtained in [Mie13, MiN14].

This model is a special case of system (2.19) by assuming that $\boldsymbol{H} = \mathbb{C}^n$ and that the dissipative variable z consists of the absolute temperatures $\theta = (\theta_1,\dots,\theta_M) \in\,]0,\infty[^M =: \mathcal{Z}_M$ of the simple heat baths, where "simple" means that the state of the heat bath is determined by a single value $\theta_j > 0$ for the absolute temperature. Thus, (2.19) reduces to an ODE with dimension n^2-1+m.

While the Poisson structure $\mathbb{J}$ on $\mathcal{Q} := \mathfrak{R}_n \times \mathcal{Z}_M$ is given by (2.11), we still have to specify the energy, the entropy, and the Onsager operator. We assume that the mth heat bath has the constant specific heat $c_m > 0$, then we have

$$\mathcal{E}(\rho,\theta) = \mathrm{tr}(\rho H) + \sum_{m=1}^M c_m\theta_m \quad\text{and}\quad \mathcal{S}(\rho,\theta) = -k_\mathrm{B}\,\mathrm{tr}(\rho\log\rho) + \sum_{m=1}^M c_m\log(\theta_m/\theta_0),$$

where $\theta_0 > 0$ is an arbitrary reference temperature. Choosing $\mathfrak{C}_m = \mathcal{C}_\rho$, the Onsager operator $\mathbb{K}$ in (2.12) is fixed by specifying $\mathrm{B}_m : \mathbb{R}^M \to \mathbb{C}^{n\times n}_{\mathrm{S}}$. We take

$$\mathrm{B}_m(\tau_1,\dots,\tau_M) = \frac{\tau_m}{c_m}H,$$

which highlights the fact that Q_m couples the quantum system to the mth heat bath. Using $\mathrm{D}_{\theta_m}\mathcal{S}(\rho,\theta)=c_m/\theta_m$ we also find $\mathrm{B}_m(z)\mathrm{D}_z\mathcal{S}(\rho,z)=H$ as desired for $(\mathrm{NIC})_2$. Hence, we define the dual entropy-production potential $\mathcal{R}^*$ via

$$\mathcal{R}^*(\rho,\theta;\mu,\tau)=\tfrac12\textstyle\sum_{m=1}^M \big\| \big[Q_m,\mu-\tfrac{\tau_m}{c_m}H\big]\big\|_{\mathcal{C}_\rho}^2+\tfrac12\tau\cdot\kappa(\theta)\tau.$$

A typical choice for $\kappa(\theta)\in\mathbb{R}_{\mathrm{S}}^{M\times M}$ is given by $\tau\cdot\kappa\tau=\sum_{m=1}^{M-1}\sum_{l=m+1}^M\widetilde{\kappa}_{ml}(\theta)\big(\frac{\tau_m}{c_m}-\frac{\tau_l}{c_l}\big)^2$, where the non-negative coefficients $\widetilde{\kappa}_{ml}(\theta)$ give the direct heat transfer between the heat baths m and l.

Setting $\mathbb{K}(\rho,\theta)=\mathrm{D}^2_{\mu,\tau}\mathcal{R}^*(\rho,\theta,0,0)$ the quintuple $(\mathfrak{R}_n\times\mathcal{Z}_M,\mathcal{E},\mathcal{S},\mathbb{J},\mathbb{K})$ defines a GENERIC system which generates the following coupled system:

$$\dot\rho\;=\jmath[\rho,H]-\sum_{m=1}^M\Big[\,Q_m\,,\,k_\mathrm{B}[Q_m,\rho]+\frac{1}{\theta_m}\mathcal{C}_\rho[Q_m,H]\,\Big],\tag{3.1a}$$

$$\dot\theta_m=\frac{1}{c_m}\sum_{l=1}^n\kappa_{ml}(\theta)\frac{c_l}{\theta_l}\;+\;\frac{1}{c_m}\langle\!\langle\,k_\mathrm{B}[Q_m,\rho]+\frac{1}{\theta_m}\mathcal{C}_\rho[Q_m,H]\,\|\,[Q_m,H]\,\rangle\!\rangle.\tag{3.1b}$$

Choosing $\kappa_{ml}(\theta)=\widehat{\kappa}_{ml}\theta_m\theta_l$ makes the first term in (3.1b). This choice is used in [GlM13] to model linear interface conditions in heterostructures using gradient structures.

Since $\dim\boldsymbol{H}=n<\infty$ the right-hand side of (3.1) is analytic in the interior of $\mathcal{Q}$, i.e. in $\operatorname{int}\mathfrak{R}\times]0,\infty[^M$, while it is continuous on $\mathcal{Q}$. Hence, solutions starting in the interior are unique as long as they stay in the interior. Even for this ODE model the global existence theory is not completely trivial. We observe that all temperatures stay bounded by energy and entropy estimates. Indeed, using $H\geq h_oI$ and $\operatorname{tr}\rho=1$ we have the upper bound

$$c_m\theta_m(t)\leq\sum_{l=1}^M c_l\theta_l(t)\leq\mathcal{E}(\rho(t),\theta(t)-h_0=\mathcal{E}(\rho(0),\theta(0))-h_0=:e_*.$$

Using the entropy we find a lower bound via

$$\begin{aligned}\mathcal{S}(\rho(0),\theta(0))\leq\mathcal{S}(\rho(t),\theta(t))&\leq k_\mathrm{B}\log n+\sum_{l=1}^M c_l\log(\theta_l(t)/\theta_0)\\&\leq k_\mathrm{B}\log n+\sum_{l\neq m}c_l\log\big(e_*/(c_l\theta_0)\big)+c_m\log(\theta_m(t)/\theta_0).\end{aligned}$$

Since $\mathfrak{R}_n$ is compact, we find that the solution $(\rho(t),\theta(t))$ stays in a compact set. Moreover, the vector field defined in (3.1) is uniformly continuous on this compact set, see (2.18) for the continuity of $\rho\mapsto\mathcal{C}_\rho$. Hence, a solution could only cease to exist by leaving the compact domain through the boundary of $\mathfrak{R}_n$. However, using the method developed for [Mie13, Thm. 21.3] it can be shown that this is not possible. Hence global existence follows, see [MiN14] for more details.

In [Mie13, Sect. 21.6] the case of one heat bath is analyzed further. In that case the single temperature $\theta=\theta_1$ can be eliminated by using energy conservation $\mathcal{E}(\rho,\theta)=E_0$ in the form $\theta=(E_0-\operatorname{tr}(\rho H))/c$. Allowing for L coupling operators Q^l connecting to one simple heat bath we arrive at the following equation for ρ alone:

$$\dot\rho=\;\jmath[H,\rho]-k_\mathrm{B}\sum_{l=1}^L\big[Q^l,[Q^l,\rho]\big]+\frac{c}{E_0-\operatorname{tr}(\rho H)}\sum_{l=1}^L\big[Q^l,\mathcal{C}_\rho[Q^l,H]\big].\tag{3.2}$$

Global existence of solutions is established in [Mie13, Thm. 21.3]. The question of uniqueness of solutions remains still open, since non-uniqueness may occur, when solutions touch the boundary of $\mathfrak{R}_n$. Additional assumptions guarantee that the thermodynamic equilibrium $\rho_{\text{eq}} = \frac{1}{Z(E_0)}\mathrm{e}^{-\beta(E_0)H}$ is the only equilibrium and that all solutions decay to this equilibrium for $t \to \infty$. Defining

$$\mu(\boldsymbol{Q}) := \inf\{\, f_{\boldsymbol{Q}}(\psi,\phi) \mid |\psi| = |\phi| = 1,\ \langle\psi|\phi\rangle = 0 \,\} \text{ where } f_{\boldsymbol{Q}}(\psi,\phi) = \sum_{l=1}^{L} |\langle Q^n\psi|\phi\rangle|^2,$$

the following result was established in [Mie13, Thm. 21.4].

Theorem 3.1 *Assume that*(3.2) *satisfies* $\mu(\boldsymbol{Q}) > 0$ *and the commutator condition*

$$\Big(A \in \mathcal{L}^2_{\mathrm{S}}(\boldsymbol{H}) \ \text{ and } \ \forall\, l = 1, ..., L\colon [Q^n, A] = 0\Big) \quad \Longrightarrow \quad \exists\, \alpha \in \mathbb{R}\colon A = \alpha I. \qquad (3.3)$$

Then, all solutions $\rho : [0,\infty[\, \to \mathfrak{R}$ *of* (3.2) *satisfy* $\rho(t) \to \rho_{\text{eq}}$.

4 A quantum dot coupled to heat equations

We consider a one-dimensional system consisting of a left reservoir and a right reservoir that are coupled to a quantum system modeling a quantum dot (QD). Our aim is to model the energy exchanges between the QD and the two reservoirs. In particular, energy can flow from one reservoir into the other only through the QD.

4.1 QD with two reservoirs

The two reservoirs are contained in the domain $\Omega = \Omega_+ \cup \Omega_-$ with $\Omega_\pm = \pm]\ell_1, \ell_3[$. We use the absolute temperature $\theta : \Omega \to]0,\infty[$ to describe the local state of the heat bath.

The quantum system is defined on the Hilbert space $\boldsymbol{H} := \mathrm{L}^2(\Omega_{\text{qm}})$ with $\Omega_{\text{qm}} :=]-\ell_2, \ell_2[$, where $0 < \ell_1 \leq \ell_2 \ll \ell_3$. We decompose this space into a subspace where the coupling may occur and the space where the quantum system is left free, namely $\boldsymbol{H} = \boldsymbol{H}_{\text{coup}} \times \boldsymbol{H}_{\text{free}}$ with $\boldsymbol{H}_{\text{coup}} = \mathrm{L}^2(\Omega_{\text{coup}})$, $\boldsymbol{H}_{\text{free}} = \mathrm{L}^2(\Omega_{\text{free}})$, $\Omega_{\text{free}} = [-\ell_1, \ell_1]$, and $\Omega_{\text{coup}} = \Omega_{\text{qm}} \backslash \Omega_{\text{free}}$. For the Hamiltonian operator H we consider the Schrödinger operator $H\psi = -\frac{1}{2m}\Psi'' + V\psi$ with a smooth potential V and boundary conditions $\psi'(\pm\ell_2) = 0$.

The total energy $\mathcal{E}$ and the total entropy $\mathcal{S}$ are given by

$$\mathcal{E}(\rho,\theta) = \mathrm{tr}(H\rho) + \int_\Omega c(x)\theta(x)\,\mathrm{d}x \text{ and } \mathcal{S}(\rho,\theta) = -k_{\mathrm{B}}\,\mathrm{tr}(\rho\log\rho) + \int_\Omega c(x)\log(\theta(x)/\theta_0)\,\mathrm{d}x.$$

While the Poisson structure $\mathbb{J}$ is given by the standard Lie-Poisson structure (2.11), we have to specify the Onsager structure in more detail. It contains the heat conduction as well as the interaction of the quantum system and the heat baths. We define it in terms of the dual dissipation potential

$$\mathcal{R}^*(\rho,\theta,\mu,\tau) = \int_\Omega \frac{k(\theta)}{2}\Big|\nabla\big(\frac{\theta}{c}\big)\Big|^2\,\mathrm{d}x + \sum_{m=1}^{M} \big|\!\big|\!\big|\, [Q_m, \mu - \mathrm{B}_m\big(\frac{\tau}{c}\big)] \,\big|\!\big|\!\big|^2_{\mathfrak{C}_\rho},$$

where $Q_m \in \mathcal{L}^\infty(\boldsymbol{H}_{\mathrm{coup}}),\ m = 1, ..., M$, are the coupling operators. For every $m \in m = 1, ..., M$ we need a linear mapping B_m from $\mathrm{L}^2(\Omega)$ into the self-adjoint operators on $\boldsymbol{H}$ such that $\mathrm{B}_m 1 = H$, e.g. a possible choice would be

$$\mathrm{B}_A v := -\frac{1}{2m} \operatorname{div}\big(\widehat{v} \nabla \psi\big) + \widehat{v} V \psi, \quad \text{where } \widehat{v}(x) = \begin{cases} v(x) & \text{for } x \in \Omega, \\ \text{affine interpolation} & \text{for } x \in [-\ell_1, \ell_1]. \end{cases}$$

The adjoint operators $\mathrm{B}_m^* : \mathcal{L}^2_{\mathrm{S}}(\boldsymbol{H}) \to \mathrm{L}^2(\Omega)$ are defined as usual, i.e. $\mathrm{tr}((\mathrm{B}_m v) A) = \int_\Omega v (\mathrm{B}_m^* A) \,\mathrm{d}x$ for all A.

Obviously, we have $\mathcal{R}^*(\rho, \theta, \mathrm{D}\mathcal{E}(\rho, \theta)) = 0$ as desired and, hence, have a GENERIC system after defining the Onsager operator $\mathbb{K}(\rho, \theta) = \mathrm{D}^2_{(\mu,\tau)} \mathcal{R}^*(\rho, \theta, 0, 0)$. To highlight the interactions between the quantum system and the heat bath we write the equations for the coupled system explicitly:

$$\begin{aligned} \dot{\rho} &= \jmath[H, \rho] - \sum_{m=1}^{M} \Big(k_{\mathrm{B}} \big[Q_m, [Q_m, \rho]\big] + \big[Q_m, \mathcal{C}_\rho [Q_m, \mathrm{B}_m(1/\theta)]\big] \Big), \\ c\dot{\theta} &= -\operatorname{div}\big(k(\theta) \nabla (1/\theta)\big) + \sum_{m=1}^{M} \mathrm{B}_m^* \big[Q_m, k_{\mathrm{B}}[Q_m, \rho] + \mathcal{C}_\rho [Q_m, \mathrm{B}_m(1/\theta)]\big], \\ 0 &= \partial_x \theta(x) \quad \text{for } x \in \partial\Omega = \{-\ell_3, -\ell_1, \ell_1, \ell_3\}. \end{aligned} \tag{4.1}$$

4.2 QD with one left and one right coupling

We now simplify the above model to highlight its structure more clearly. For this we making particular choices, namely $M = 2$ such that $Q_- = Q_1$ couples to the left reservoir and $Q_+ = Q_2$ couples to the right. In particular, we assume $Q_\pm = g_\pm \otimes \overline{g}_\pm$ with $\mathrm{supp}(g_\pm) \subset \pm[\ell_1, \ell_2]$ and $g_\pm \in \mathrm{H}^2_0(\overline{\Omega}_{\mathrm{coup}})$ such that $Hg_\pm$ lies in $\mathrm{L}^2(\Omega)$ and $\jmath[Q_\pm, H] \in \mathcal{L}^2_{\mathrm{S}}(\boldsymbol{H})$. Finally, we choose $\mathrm{B}_\pm$ as simple as possible, namely

$$\mathrm{B}_\pm(v) = \llbracket v \rrbracket_\pm H \quad \text{with } \llbracket v \rrbracket_\pm = \frac{1}{\ell_2 - \ell_1} \int_{\pm[\ell_1, \ell_2]} v(y) \,\mathrm{d}y,$$

where in the case $\ell_1 = \ell_2$ the value $\llbracket v \rrbracket_\pm$ can be interpreted as a point evaluation $v(\pm \ell_1)$. Hence, B_+ sees the average temperature on the right coupling region, while B_- that on the left. In particular, the adjoints $\mathrm{B}_\pm^*$ are simple as well, namely $\mathrm{B}_\pm^* Q = \mathbb{1}_{\pm[\ell_1, \ell_2]} \,\mathrm{tr}(QH)$, where $\mathbb{1}_S$ denotes the indicator function for the set S.

With these choices (4.1) takes the more specific form

$$\begin{aligned} \dot{\rho} &= \jmath[H, \rho] - \sum_{\alpha \in \{+,-\}} \Big(k_{\mathrm{B}} \big[Q_\alpha, [Q_\alpha, \rho]\big] + \llbracket 1/\theta \rrbracket_\alpha \big[Q_\alpha, \mathcal{C}_\rho [Q_\alpha, H]\big] \Big), \\ c\dot{\theta} &= \operatorname{div}\big(\frac{k(\theta)}{\theta^2} \nabla \theta\big) + \sum_{\alpha \in \{+,-\}} \frac{\mathbb{1}_{\alpha[\ell_1, \ell_2]}}{\ell_2 - \ell_1} \,\mathrm{tr}\, \Big([Q_\alpha, H] \big(k_{\mathrm{B}} [Q_\alpha, \rho] + \llbracket 1/\theta \rrbracket_\alpha \mathcal{C}_\rho [Q_\alpha, H] \big) \Big), \end{aligned} \tag{4.2}$$

plus the same boundary conditions for θ as in (4.1). In (4.2) we nicely see the coupling between the heat equation and the quantum system: the dissipative terms in the quantum system give rise to a source term in the heat equation. The GENERIC structure guarantees that the energy remains constant, while the entropy increases.

4.3 Non-equilibrium steady states and fluxes

The above model allows us to study non-equilibrium steady states (NESS) by assuming that the reservoirs are huge. Mathematically we realize this by making the specific heat c very large, namely $c = 1/\varepsilon$ for $\varepsilon \searrow 0$. For a fix ε we still expect that all solutions (ρ, θ) will converge to the thermodynamic equilibrium. However, starting from initial conditions (ρ, θ), where $\theta(x) = \widehat{\theta}_\pm$ for $x \in \pm[\ell_1, \ell_3]$, one expects that ρ decays to an equilibrium on a time-scale of order 1 (relative to ε), while the temperatures only change with a rate proportional to ε. Hence, we can formulate a nonlinear equation for the NESS $\widehat{\rho}$ as follows:

$$0 = \jmath[H, \widehat{\rho}] - \sum_{\alpha \in \{+,-\}} \Big(k_\mathrm{B}\big[Q_\alpha, [Q_\alpha, \widehat{\rho}]\big] + \frac{1}{\widehat{\theta}_\alpha}\big[Q_\alpha, \mathcal{C}_{\widehat{\rho}}[Q_\alpha, H]\big] \Big). \tag{4.3}$$

Here the NESS $\widehat{\rho}$ is the only unknown, since the temperatures $\widehat{\theta}_+$ and $\widehat{\theta}_-$ are given.

The heat equation is no longer part of the problem, however it allows us to calculate the energy flux through the quantum system. The energies in the left and the right reservoirs are given by $\int_{\pm[\ell_1,\ell_3]} \frac{1}{\varepsilon}\theta(x)\,\mathrm{d}x$. Taking the time derivative of these terms and inserting the heat equation we obtain the flux from the left to the right reservoir by

$$\begin{aligned} &\mathcal{F}(\widehat{\theta}_-, \widehat{\theta}_+) := \mathcal{F}_+(\widehat{\theta}_-, \widehat{\theta}_+) - \mathcal{F}_-(\widehat{\theta}_-, \widehat{\theta}_+) \\ &\text{with } \mathcal{F}_\pm(\widehat{\theta}_-, \widehat{\theta}_+) := \mathrm{tr}\,\Big([Q_\pm, H]\big(k_\mathrm{B}[Q_\pm, \widehat{\rho}] + \frac{1}{\widehat{\theta}_\pm}\mathcal{C}_{\widehat{\rho}}[Q_\pm, H]\big)\Big), \end{aligned} \tag{4.4}$$

where the NESS $\widehat{\rho}$ is a function of $(\widehat{\theta}_-, \widehat{\theta}_+)$. The term $\mathrm{div}\,\big(k\nabla(1/\theta)\big)$ does not contribute to the flux terms $\mathcal{F}_\pm$, because of the no-flux boundary conditions. It is interesting to see that the non-equilibrium flux does not depend on the choice of the operators $\mathrm{B}_\pm$.

For $\widehat{\theta}_\pm = \theta_*$ one obtains the thermodynamical equilibrium $\widehat{\rho} = \rho_\mathsf{eq} = \frac{1}{Z}\mathrm{e}^{-\beta H}$ with $\beta = 1/(k_\mathrm{B}\theta)$. Assuming $\widehat{\theta} = \theta_* \pm \delta$ it should be possible to calculate $\widehat{\rho}(\delta) = \rho_\mathsf{eq} + \delta\sigma + O(\delta^2)$ and to find an expansion for the non-equilibrium flux $\mathcal{F}(\theta_* - \delta, \theta_* + \delta) = \delta F_1 + O(\delta^2)$, where we expect that F_1 can be related to the Landauer-Büttiker theory, see e.g. [CNZ09].

5 Thermo-opto-electronic models for semiconductors

The coupling of quantum systems to classical opto-electronic systems is common practice in the modeling of laser devices, if the optically active zones are based on quantum wells or quantum dots, see e.g. [KW*11]. Fully quantum mechanical models as in [NWZ13] cannot be used because of the macroscopic complexity of real semiconductor devices. Hence, such models have to consist of two subparts that are typically considered independently. On the one hand the drift-diffusion equation for the charged particles (usually free electrons and holes in a semiconductor crystal) and the heat equation form a parabolic system that can be written as a gradient system $\dot{q} = \mathbb{K}(q)\mathrm{D}\mathcal{S}(q)$, see [Mie11b]. On the other hand the Maxwell-Bloch system for the electromagnetic fields and the polarization form a hyperbolic system that is mostly treated as an energy conserving Hamiltonian system which contains a quantum model, see [JMR00, Dum05]. We present the main results of [BKM14], which show that both models can be coupled via GENERIC.

5.1 The Maxwell-Bloch equation as Hamiltonian system

Finally, we present an example of a coupling between a quantum system and a classical system, where the quantum system is distributed in the whole crystal, but this time it is described by a finite-dimensional Hilbert space $\boldsymbol{H} = \mathrm{C}^n$ on each material point x in the domain $\Omega \subset \mathbb{R}^3$. We assume that there is no coupling between the different points, which is a good approximation for certain polarizations of an optically active crystal.

To introduce the notation we start with Maxwell's equations in the vacuum $\mathbb{R}^3$ by considering the dielectric displacement $\boldsymbol{D}$ and the magnetic flux $\boldsymbol{B}$ as the basic fields:

$$\dot{\boldsymbol{D}} = \operatorname{curl} \boldsymbol{H}, \quad \dot{\boldsymbol{B}} = -\operatorname{curl} \boldsymbol{E}, \quad \operatorname{div} \boldsymbol{D} = 0 = \operatorname{div} \boldsymbol{B}$$

with conserved total energy $\mathcal{E}_\mathrm{M}(\boldsymbol{D}, \boldsymbol{B}) = \int_{\mathbb{R}^3} \frac{1}{2\varepsilon_0}|\boldsymbol{D}|^2 + \frac{1}{2\mu_0}|\boldsymbol{B}|^2 \,\mathrm{d}x$, electric field $\boldsymbol{E} = \mathrm{D}_{\boldsymbol{D}}\mathcal{E}_\mathrm{M}(\boldsymbol{D}, \boldsymbol{B}) = \frac{1}{\varepsilon_0}\boldsymbol{D}$, and magnetic field $\boldsymbol{H} = \mathrm{D}_{\boldsymbol{B}}\mathcal{E}_\mathrm{M}(\boldsymbol{D}, \boldsymbol{B}) = \frac{1}{\mu_0}\boldsymbol{B}$.

The Maxwell-Bloch system is a combination of the Maxwell equations and an n-level quantum system at each material point $x \in \Omega$ described by the density matrix $\rho(t, x) \in \mathfrak{R}_n := \mathfrak{R} \cap \mathbb{C}^{n\times n}_{\mathrm{Herm}}$. This quantum system contains the material properties of the underlying crystal Ω. Without interaction with the electromagnetic waves it is given via $\dot\rho = \jmath[\rho, N_\mathrm{B}]$ where $N_\mathrm{B} = N_\mathrm{B}^* \in \mathbb{C}^{n\times n}$ is the Bloch Hamiltonian. The coupling of ρ to Maxwell's equation occurs via the polarization in the form $\boldsymbol{D} = \boldsymbol{E} + \boldsymbol{P}$ with polarization $\boldsymbol{P}(t, x) = \Gamma\rho(t, x)$ where $\Gamma : \mathbb{C}^{n\times n}_{\mathrm{Herm}} \to \mathbb{R}^3$ is called the dipole-moment operator. Thus we arrive at the nonlinear Maxwell-Bloch system

$$\dot{\boldsymbol{D}} = \operatorname{curl} \boldsymbol{H}, \qquad \dot{\boldsymbol{B}} = -\operatorname{curl}(\boldsymbol{D}-\Gamma\rho), \qquad \dot\rho = \jmath[\rho, N_\mathrm{B}-\Gamma^*(\boldsymbol{D}-\Gamma\rho)]. \tag{5.1}$$

Choosing the space $\boldsymbol{Q} = \mathrm{L}^2(\Omega, \operatorname{div})^3 \times \mathrm{L}^2(\Omega, \operatorname{div})^3 \times \mathfrak{R}_n$ and setting $\varepsilon_0 = \mu_0 = 1$ for simplicity, these equations form a Hamiltonian $(\boldsymbol{Q}, \mathcal{E}, \mathbb{J})$ with the energy $\mathcal{E}(\boldsymbol{D}, \boldsymbol{B}, \rho) = \int_\Omega \frac{1}{2\varepsilon_0}|\boldsymbol{D}-\Gamma\rho|^2 + \frac{1}{2\mu_0}|\boldsymbol{B}|^2 + \operatorname{tr}(N_\mathrm{B}\rho)\,\mathrm{d}x$ as follows

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \boldsymbol{D} \\ \boldsymbol{B} \\ \rho \end{pmatrix} = \mathbb{J}(\rho)\begin{pmatrix} \mathrm{D}_{\boldsymbol{D}}\mathcal{E} \\ \mathrm{D}_{\boldsymbol{B}}\mathcal{E} \\ \mathrm{D}_\rho\mathcal{E} \end{pmatrix} \quad \text{where } \mathbb{J}(\rho) = \begin{pmatrix} 0 & \operatorname{curl} & 0 \\ -\operatorname{curl} & 0 & 0 \\ 0 & 0 & \jmath[\rho, \Box] \end{pmatrix}.$$

In [JMR00, Dum05] the variables $(\boldsymbol{E}, \boldsymbol{H}, \rho)$ are used which lead to a slightly more involved formulation for the Poisson structure $\mathbb{J}$, but make the analysis easier.

5.2 Energy-drift-diffusion systems as Onsager system

As is explained in [Mie11b], one can also handle general energy-drift-diffusion systems with reactions as treated in [AGH02] as long as the reaction satisfy a detailed balance condition. The formulation is most easily in terms of the densities of the charge carriers, namely $\boldsymbol{c}(t, x) \in [0, \infty[^I$, and the density $u \in \mathbb{R}$ of the internal energy. Then, the total energy $\mathcal{E}$ and the total entropy $\mathcal{S}$ are given by

$$\mathcal{E}(\boldsymbol{c}, u) = \int_\Omega \frac{\varepsilon}{2}|\nabla\phi_{\boldsymbol{c}}|^2 + u\,\mathrm{d}x \quad \text{and} \quad \mathcal{S}(c, u)\,\mathrm{d}x,$$

where the electrostatic potential $\phi_{\boldsymbol{c}}$ is the unique solution of the Poisson equation

$$-\operatorname{div}\big(\varepsilon\nabla\phi\big) = \delta_{\mathrm{dop}} + \boldsymbol{z}\cdot\boldsymbol{c} \text{ in } \Omega, \text{ plus suitable bound. cond.,}$$

where $\boldsymbol{z} = (z_1, .., z_I) \in \mathbb{Z}^I$ is the vector of the charge numbers. We note that the differentials of the these functionals have the form

$$\mathrm{D}\mathcal{E}(\boldsymbol{c}, u) = \begin{pmatrix} \phi_{\boldsymbol{c}} \boldsymbol{z} \\ 1 \end{pmatrix} \quad \text{and} \quad \mathrm{D}\mathcal{S}(\boldsymbol{c}, u) = \begin{pmatrix} \partial_{\boldsymbol{c}} S(\boldsymbol{c}, u) \\ \partial_u S(\boldsymbol{c}, u) \end{pmatrix} \text{ where } \partial_u S(\boldsymbol{c}, u) = 1/\theta.$$

We define the Onsager operator $\mathbb{K}$ in terms of the dual entropy-production potential

$$\mathcal{R}^*(\boldsymbol{c}, u; \boldsymbol{\mu}, \tau) = \frac{1}{2} \int_\Omega \begin{pmatrix} \nabla\mu - \tau \boldsymbol{z} \otimes \nabla \phi_{\boldsymbol{c}} \\ \nabla \tau \end{pmatrix} : \mathbb{M}(\boldsymbol{c}, u) : \begin{pmatrix} \nabla\mu - \tau \boldsymbol{z} \otimes \nabla \phi_{\boldsymbol{c}} \\ \nabla \tau \end{pmatrix} + \boldsymbol{\mu} \cdot \mathbb{H}(\boldsymbol{c}, u) \boldsymbol{\mu} \, \mathrm{d}x,$$

i.e. $\mathbb{K} = \mathrm{D}^2_{\boldsymbol{\mu},\tau} \mathcal{R}^*$. Here $\mathbb{M}$ gives the mobilities of the particles and the heat conduction, while $\mathbb{H}$ gives the reaction coefficients.

By construction we have $\Psi^*(\boldsymbol{c}, u; \mathrm{D}\mathcal{E}(\boldsymbol{c}, u)) \equiv 0$, which implies energy conservation for the Onsager system via $\mathbb{K}(\boldsymbol{c}, u) \mathrm{D}\mathcal{E}(\boldsymbol{c}, u) \equiv 0$. The Onsager evolution $\frac{\mathrm{d}}{\mathrm{d}t} \binom{\boldsymbol{c}}{u} = \mathbb{K}(\boldsymbol{c}, u) \mathrm{D}\mathcal{S}(\boldsymbol{c}, u)$ is then given in the form

$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} \boldsymbol{c} \\ u \end{pmatrix} + \begin{pmatrix} \operatorname{div} \boldsymbol{J}_{\boldsymbol{c}} \\ \operatorname{div} \boldsymbol{j}_u \end{pmatrix} = - \begin{pmatrix} 0 \\ \boldsymbol{z} \otimes \nabla \phi_{\boldsymbol{c}} : \boldsymbol{J}_{\boldsymbol{c}} \end{pmatrix} + \begin{pmatrix} \mathbb{H}(\boldsymbol{c}, u) \partial_{\boldsymbol{c}} S(\boldsymbol{c}, u) \\ 0 \end{pmatrix} \tag{5.2}$$

$$\text{where } \begin{pmatrix} \boldsymbol{J}_{\boldsymbol{c}} \\ \boldsymbol{j}_u \end{pmatrix} = \mathbb{M}(\boldsymbol{c}, u) \begin{pmatrix} \nabla \partial_{\boldsymbol{c}} S(\boldsymbol{c}, u) - \partial_u S(\boldsymbol{c}, u) \boldsymbol{z} \otimes \nabla \phi_{\boldsymbol{c}} \\ \nabla \partial_u S(\boldsymbol{c}, u) \end{pmatrix}.$$

The equation for u in (5.2) contains the work of the charge carriers moving against the electric field $\boldsymbol{E} = \nabla \phi_{\boldsymbol{c}}$, namely $\boldsymbol{E} \cdot (\boldsymbol{z} \cdot \boldsymbol{J}_{\boldsymbol{c}})$, where $\boldsymbol{z} \cdot \boldsymbol{J}_{\boldsymbol{c}}$ is the net flux of all moving charges. This term is needed in the energy balance to compensate for the change in the electrostatic energy $\frac{\varepsilon}{2} |\nabla \phi_{\boldsymbol{c}}|^2$.

5.3 A GENERIC formulation for thermo-opto-electronics

To couple the Maxwell-Bloch equation and the energy-drift-diffusion system we use the state variable $q = (\boldsymbol{D}, \boldsymbol{B}, \rho, \boldsymbol{c}, u) : \Omega \to \mathbb{R}^3 \times \mathbb{R}^3 \times \mathfrak{R}_n \times [0, \infty[^I \times \mathbb{R}$. If $S(\boldsymbol{D}, \boldsymbol{B}, \rho, \boldsymbol{c}, u)$ is the entropy density then $\partial_u S$ gives the inverse $1/\theta$ of the temperature θ. The total energy $\mathcal{E}$ and the total entropy $\mathcal{S}$ are assumed to have the form

$$\mathcal{E}(q) = \int_\Omega \frac{1}{2} |\boldsymbol{D} - \Gamma \rho|^2 + \frac{1}{2} |\boldsymbol{B}|^2 + \operatorname{tr}(N_\mathrm{B} \rho) + u \, \mathrm{d}x, \quad \mathcal{S}(q) = \int_\Omega S(\rho, \boldsymbol{c}, u) \, \mathrm{d}x$$

leading to the thermodynamic driving forces

$$\begin{pmatrix} \boldsymbol{E} \\ \boldsymbol{H} \\ \eta \\ \boldsymbol{\mu} \\ \tau \end{pmatrix} = \mathrm{D}\mathcal{E}(q) = \begin{pmatrix} \boldsymbol{D} - \Gamma \rho \\ \boldsymbol{B} \\ \Gamma^*(\Gamma \rho - \boldsymbol{D}) + N_\mathrm{B} \\ 0 \\ 1 \end{pmatrix}, \quad \mathrm{D}\mathcal{S}(q) = \begin{pmatrix} 0 \\ 0 \\ \partial_\rho S \\ \partial_{\boldsymbol{c}} S \\ \partial_u S \end{pmatrix}.$$

For the Poisson structure we choose an operator that is similar to the Maxwell-Bloch operator, but is now augmented by a term that accounts for reversible exchanges of heat (also called latent heat in mechanics):

$$\mathbb{J}_{\mathrm{TOE}}(q) := \begin{pmatrix} 0 & \operatorname{curl} & 0 & 0 & 0 \\ -\operatorname{curl} & 0 & 0 & 0 & 0 \\ 0 & 0 & \jmath[\rho, \square] & 0 & -\mathcal{A}(q) \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathcal{A}(q)^* & 0 & 0 \end{pmatrix}$$

with $\mathcal{A}(q)\tau = \jmath\,\tau\,\theta\,[\rho, \partial_\rho S(q)]$ and $\mathcal{A}(q)^*\eta = \jmath\theta\,\mathrm{tr}\,\big(\eta[\rho, \partial_\rho S(q)]\big)$, cf. [Mie11a] for similar latent heat terms in thermoelasticity. Here $\mathcal{A}$ is constructed in such a way that to obtain $(\mathrm{NIC})_1$ holds, namely using $\theta\partial_u S \equiv \mathbb{1}$ we find $\mathbb{J}_{\mathrm{TOE}}(q)\mathrm{D}\mathcal{S}(q) = 0$. Hence, the reversible part of the dynamics of the density matrix ρ takes the form

$$\dot{\rho} = \jmath\big[\rho,\, \mathrm{D}_\rho\mathcal{E}(q) - \theta\mathrm{D}_\rho\mathcal{S}(\rho)\big] = \jmath\big[\rho,\, \mathrm{D}_\rho\mathcal{F}(\rho)\big] \tag{5.3}$$

which emphasizes the rôle of the free energy $\mathcal{F} = \mathcal{E} - \theta{*}\mathcal{S}$ for the reversible dynamics.

The Onsager operator $\mathbb{K}_{\mathrm{TOE}}$ for thermo-opto-electronic has the additive form:

$$\mathbb{K}_{\mathrm{TOE}}(q) = \mathbb{K}_{\mathrm{react}}(q) + \mathbb{K}_{\mathrm{B}}(q) + \mathbb{K}_{\mathrm{diff}}(q) + \mathbb{K}_{\mathrm{heat}}(q),$$

where each term is of the form $\mathbb{K}_j(q) = \mathbb{A}_j(q)^*\mathbb{L}_j(q)\mathbb{A}_j(q)$ with $\mathbb{L}_j \geq 0$. Hence if $\mathbb{A}_j(q)\mathrm{D}\mathcal{E}(q) \equiv 0$ holds for all j then $(\mathrm{NIC})_2$ holds as well.

(i) For the *reactions* between charge carriers (including stimulated emission) we choose $\mathbb{A}_{\mathrm{react}}(q)(\boldsymbol{E}, \boldsymbol{H}, \eta, \boldsymbol{\mu}, \tau) = \boldsymbol{\mu}$ and $\mathbb{L}_{\mathrm{react}} = \mathbb{H}$. Moreover, $\mathbb{A}_{\mathrm{react}}(q)\mathrm{D}\mathcal{E}(q) \equiv 0$ follows from $\mathrm{D}_{\boldsymbol{c}}\mathcal{E}(q) \equiv 0$. We obtain $\mathbb{K}_{\mathrm{react}}(q)\mathrm{D}\mathcal{S}(q) = \big(0, 0, 0, \mathbb{H}\mathrm{D}_{\boldsymbol{c}}\mathcal{S}(q), 0\big)^{\mathsf{T}}$.

(ii) To model the *quantum relaxations* we set $N(q) := \mathrm{D}_\rho\mathcal{E}(q) = N_{\mathrm{B}} - \Gamma^*(\boldsymbol{D}{-}\Gamma\rho)$, define $\mathbb{A}_{\mathrm{B}}(q)(\boldsymbol{E}, \boldsymbol{H}, \eta, \boldsymbol{\mu}, \tau) := \eta - \tau N(q)$, and choose an arbitrary $\mathbb{L}(q) \geq 0$, e.g. $\mathbb{L}(q)\eta = \sum_{m=1}^{M}\big[Q_m, \mathcal{C}_\rho[Q_m, \eta]\big]$. Using the definition of $N(q)$ and $\mathrm{D}_\tau\mathcal{E}(q) = 1$ gives $\mathbb{A}_{\mathrm{B}}(q)\mathrm{D}\mathcal{E}(q) \equiv 0$, and $(\mathrm{NIC})_2$ holds. In particular, we obtain

$$\mathbb{K}_{\mathrm{B}}(q)\mathrm{D}\mathcal{S}(q) = \Big(0, 0, \mathbb{L}(q)\big(\partial_\rho S(q) - \tfrac{1}{\theta}N(q)\big), 0, -\,\mathrm{tr}\,\big(N(q)\mathbb{L}(\partial_\rho S(q) - \tfrac{1}{\theta}N(q))\big)\Big)^{\mathsf{T}}.$$

We observe that the dissipative relaxations are driven by the *free entropy* $\mathcal{N}$, namely by $\mathrm{D}_\rho\mathcal{N}(q) = \mathrm{D}_\rho\mathcal{S}(q) - \frac{1}{\theta}\mathrm{D}_\rho\mathcal{E}(q)$. Moreover, the last term can be seen as a heating term due to dissipation in the quantum systems.

(iii) The *drift and the diffusion* of the charge carriers is modeled via the mobility. Since the flux tensor $\boldsymbol{J_c}$ for the densities $\boldsymbol{c}$ should have the form $\boldsymbol{J_c} = \mathbb{M}_{\boldsymbol{c}}(\nabla\boldsymbol{\mu} - \frac{1}{\theta}\boldsymbol{z}{\otimes}\boldsymbol{E}) \in \mathbb{R}^{I\times d}$ we define the operator $\mathbb{A}_{\mathrm{mob}}(q)(\boldsymbol{E}, \boldsymbol{H}, \eta, \boldsymbol{\mu}, \tau)^{\mathsf{T}} := \boldsymbol{z}{\otimes}\boldsymbol{E} + \nabla\boldsymbol{\mu} - \tau\,\boldsymbol{z}{\otimes}(\boldsymbol{D}{-}\Gamma\rho) \in \mathbb{R}^{I\times d}$. Using $\boldsymbol{E} = \boldsymbol{D}{-}\Gamma\rho$ we find the relations

$$\mathbb{A}_{\mathrm{mob}}(q)\mathrm{D}\mathcal{E}(q) \equiv 0, \qquad \mathbb{A}_{\mathrm{mob}}(q)\mathrm{D}\mathcal{S}(q) = \nabla\partial_{\boldsymbol{c}}S - \frac{1}{\theta}\boldsymbol{z}{\otimes}(\boldsymbol{D}{-}\Gamma\rho).$$

Thus, $\mathbb{K}_{\mathrm{mob}}(q) = \mathbb{A}(q)^*\mathbb{M}_{\boldsymbol{c}}(q)\mathbb{A}(q)$ satisfies $(\mathrm{NIC})_2$ and provides

$$\mathbb{K}_{\mathrm{diff}}(q)\mathrm{D}\mathcal{S}(q) = \begin{pmatrix} \boldsymbol{z}{\cdot}\mathbb{M}_{\boldsymbol{c}}(\nabla\boldsymbol{\mu}{-}\frac{1}{\theta}\boldsymbol{z}{\otimes}\boldsymbol{E}) \\ 0 \\ 0 \\ -\,\mathrm{div}\,\big(\mathbb{M}_{\boldsymbol{c}}(\nabla\boldsymbol{\mu}{-}\frac{1}{\theta}\boldsymbol{z}{\otimes}\boldsymbol{E})\big) \\ (\boldsymbol{z}{\otimes}\boldsymbol{E}){:}\mathbb{M}_{\boldsymbol{c}}(\nabla\boldsymbol{\mu}{-}\frac{1}{\theta}\boldsymbol{z}{\otimes}\boldsymbol{E}) \end{pmatrix}$$

The first component gives the effective charge flux $\boldsymbol{z}{\cdot}\boldsymbol{J_c}$, the fourth component generates the drift and the diffusion term, and the fifth component contains the power of charges working against the electric field.

(iv) The heat transfer can be given in the form

$$\mathbb{K}_{\mathrm{heat}}(q)(\boldsymbol{E}, \boldsymbol{H}, \eta, \boldsymbol{\mu}, \tau)^{\mathsf{T}} = \big(0, 0, 0, 0, -\,\mathrm{div}\,\big(\kappa(q)\nabla\tau\big)\big)^{\mathsf{T}}.$$

Clearly $\mathrm{D}_u\mathcal{E}(q) = 1$ gives $\mathbb{K}_{\mathrm{heat}}(q)\mathrm{D}\mathcal{E}(q) = 0$, which is $(\mathrm{NIC})_2$. In fact, in general we may allow for cross-diffusion between charges and heat:

$$\begin{pmatrix} \boldsymbol{J_c} \\ \boldsymbol{j}_u \end{pmatrix} = \begin{pmatrix} \mathbb{M}_{\boldsymbol{c}} & \mathbb{M}_{\mathrm{cross}} \\ \mathbb{M}_{\mathrm{cross}}^* & \kappa(q) \end{pmatrix} \begin{pmatrix} \mathbb{A}_{\mathrm{mob}}(q)\mathrm{D}\mathcal{S}(q) \\ \nabla\partial_u S(q) \end{pmatrix}. \tag{5.4}$$

Now we are able to write the full GENERIC system $\dot q = \mathbb{J}_{\mathrm{TOE}}(q)\mathrm{D}\mathcal{E}(q) + \mathbb{K}_{\mathrm{TOE}}(q)\mathrm{D}\mathcal{S}(q)$ with the building blocks described above. It leads to the following coupled system of partial differential equations

$$
\begin{aligned}
\dot{\boldsymbol{D}} &= \quad \operatorname{curl}\boldsymbol{B} && +\boldsymbol{z}\boldsymbol{\cdot}\boldsymbol{J}_{\boldsymbol{c}},\\
\dot{\boldsymbol{B}} &= -\operatorname{curl}\boldsymbol{E}, &&\\
\dot\rho &= \jmath\big[\,\rho\,,\,N(q) - \theta\partial_\rho S(q)\big] && +\mathbb{L}(q)\big(\partial_\rho S(q) - \tfrac{1}{\theta}N(q)\big),\\
\dot{\boldsymbol{c}} &= && -\operatorname{div}\boldsymbol{J}_{\boldsymbol{c}} + \mathbb{H}(q)\partial_{\boldsymbol{c}}S(\rho,\boldsymbol{c},u),\\
\dot u &= \theta\,\mathrm{tr}\,\big(N(q)\mathrm{i}[\rho,\partial_\rho S(q)]\big) - \operatorname{div}\boldsymbol{j}_u - \mathrm{tr}\,\Big(N(q)\mathbb{L}(q)\big(\partial_\rho S(q) - \tfrac{1}{\theta}N(q)\big)\Big) + (\boldsymbol{z}\otimes\boldsymbol{E})\boldsymbol{:}\boldsymbol{J}_{\boldsymbol{c}}, &&
\end{aligned}
$$

where $(\boldsymbol{J}_{\boldsymbol{c}}, \boldsymbol{j}_u)$ is given in (5.4), $\boldsymbol{E} = \boldsymbol{D} - \Gamma\rho$, and $N(q) = \mathrm{D}_\rho\mathcal{E}(q) = N_{\mathrm{B}} - \Gamma^*(\boldsymbol{D} - \Gamma\rho)$.

The first equation (combined with the fourth and using the charge neutrality $\boldsymbol{z}\boldsymbol{\cdot}\mathbb{H} \equiv 0$ of the reactions) is compatible with $\operatorname{div}\boldsymbol{D} = \delta_{\mathrm{dop}} + \boldsymbol{z}\boldsymbol{\cdot}\boldsymbol{c}$ for all $t > 0$, if it is satisfied for $t = 0$. The last equation can be written as

$$
\begin{aligned}
\dot u &= -\operatorname{div}\boldsymbol{j}_u + (\boldsymbol{z}\otimes\boldsymbol{E})\boldsymbol{:}\boldsymbol{J}_{\boldsymbol{c}} - \mathrm{tr}\,\Big(N(q)\big(\jmath[\rho, \mathrm{D}_\rho\mathcal{E} - \theta\mathrm{D}_\rho\mathcal{S}] + \mathbb{L}(q)(\mathrm{D}_\rho\mathcal{S} - \tfrac{1}{\theta}\mathrm{D}_\rho\mathcal{E})\big)\Big)\\
&= -\operatorname{div}\boldsymbol{j}_u + \boldsymbol{E}\cdot\boldsymbol{z}\boldsymbol{\cdot}\boldsymbol{J}_{\boldsymbol{c}} - \mathrm{tr}\,\big(\mathrm{D}_\rho\mathcal{E}(q)\dot\rho\big),
\end{aligned}
$$

which displays the balance of internal energy with the work of the charges against the electric field $\boldsymbol{E}$ and the work of the quantum system. For more details see [BKM14].

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