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Dissipative quantum mechanics using GENERIC

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Abstract

Pure quantum mechanics can be formulated as a Hamiltonian system in terms of 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 (General Equations for Non-Equilibrium Reversible Irreversible Coupling) to construct thermodynamically consistent evolution equations as a sum of a Hamiltonian and a gradient-flow contribution, which satisfy a particular non-interaction condition:

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

One of our models couples a quantum system to a finite number of heat baths each of which is described by a time-dependent temperature.

The dissipation mechanism is modeled via the canonical correlation operator, which is the inverse of the Kubo-Mori metric for density matrices and which is strongly linked to the von Neumann entropy for quantum systems. Thus, one recovers the dissipative double-bracket operators of the Lindblad equations but encounters a correction term for the consistent coupling to the dissipative dynamics.

For the finite-dimensional and isothermal case we provide a general existence result and discuss sufficient conditions that guarantee that all solutions converge to the unique thermal equilibrium state.

Finally, we compare of our gradient flow formulation for quantum systems with the Wasserstein gradient flow formulation for the Fokker-Planck equation and the entropy gradient flow formulation for reversible Markov chains.

1 Introduction

A fundamental problem in nanoscience is a consistent coupling of quantum mechanics with effects on larger scales. 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 are still satisfied. We follow [Ött10, Ött11] in modeling the coupling between classical dissipative systems and reversible quantum systems. The basis is the theory of GENERIC systems, which stands for the acronym General Equations for Non-Equilibrium Reversible Irreversible Coupling. It provides systems that are thermodynamically correct in the sense that the total energy is preserved while the total entropy is nondecreasing. Moreover, the evolution has an additive split into the reversible dynamics driven by a co-symplectic structure (Poisson bracket) acting on the energy and the irreversible dynamics given as a gradient flow with the total entropy as the driving functional.

Evolution of the quantum mechanical system is given in terms of the density matrix $\rho = \rho^* \geq 0$ such that it can be coupled to more macroscopic dissipative components z. Thus, the total state $q = (\rho, z)$ lies in the state space $\mathcal{Q} = \mathfrak{R} \times Z$, and the evolution is given by the GENERIC system

$(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathcal{J}, \mathcal{K})$. Here $\mathcal{E}$ and $\mathcal{S}$ are the conserved energy functional and the entropy functional. The mapping $\mathcal{J}$ defines a Poisson structure, i.e. $\mathcal{J}(q) = -\mathcal{J}(q)^*$ and the Jacobi identity holds, while $\mathcal{K}$ defines an Onsager structure, i.e. $\mathcal{K}(q) = \mathcal{K}(q)^* \geq 0$. The evolution is given in the form

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

where the crucial structural condition is the mutual ***non-interaction condition***

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

We discuss the main properties of GENERIC systems in Section 2. For the history and the motivation of the GENERIC framework we refer to [GrÖ97, ÖtG97, Ött05, Grm10]. For applications in continuum mechanics see [Mie11a].

In this work we follow the approach pioneered in [Ött10, Ött11] and analyze the system proposed there mathematically. Our aim is to provide existence results as well as conditions guaranteeing that the solutions converge into thermal equilibrium. To be more precise we consider GENERIC systems where the coupling occurs only through the Onsager operator $\mathcal{K}$. We assume that $\mathcal{E}$, $\mathcal{S}$, and $\mathcal{J}$ have the form

$$\mathcal{E}(\rho, z) = \langle\!\langle\, \rho \,\|\, H \,\rangle\!\rangle + E(z),\ \mathcal{S}(\rho, z) = -k_{\mathrm{B}}\langle\!\langle\, \rho \,\|\, \log \rho \,\rangle\!\rangle + S(z),\ \mathcal{J}(q, z) = \begin{pmatrix} \jmath[\rho, \square] & 0 \\ 0 & 0 \end{pmatrix},$$

where $\jmath = \mathrm{i}/\hbar$ and "$\square$" indicates the slot where the argument should be inserted. Here $\langle\!\langle\, A \,\|\, B \,\rangle\!\rangle$ denotes the operator scalar product which for $A, B \in \mathbb{C}^{N\times\mathbb{N}}$ turns into $\langle\!\langle\, A \,\|\, B \,\rangle\!\rangle = \sum_{j,k=1}^{N} A_{jk}\overline{B}_{jk} = \mathrm{tr}(AB^*)$. Hence $-k_{\mathrm{B}}\langle\!\langle\, \rho \,\|\, \log \rho \,\rangle\!\rangle$ is the quantum mechanical von Neumann entropy whereas $S(z)$ is assumed to be a concave macroscopic entropy.

The coupling between the components ρ and z occurs through $\mathcal{K}$ which is most easily formulated in terms of the dual dissipation potential $\Psi^*(q;\xi) = \frac{1}{2}\langle \mathcal{K}(q)\xi, \xi\rangle$ and is assumed to have the form

$$\Psi^*(\rho, z; \eta, \zeta) = \frac{1}{2}\sum_{n=1}^{N} \| \left[Q_n(z), \eta - \langle \alpha_n(z), \zeta\rangle H\right] \|^2_{\boldsymbol{C}_j(\rho,z)},$$

where $Q_n(z)$, $j = 1, .., N$ are coupling operators and $\|A\|^2_{\boldsymbol{C}} := \langle\!\langle\, \boldsymbol{C}A \,\|\, A \,\rangle\!\rangle$. The dissipative coupling via Q, and hence the interaction of the quantum system with the z component, occurs only through the commutators

$$[Q, \Xi] := Q\,\Xi \,-\, \Xi\,Q.$$

The coefficients α_m are assumed to satisfy the relation $\langle \alpha_n(z), \mathrm{D}E(z)\rangle \equiv 1$ such that $\Psi^*(q, \mathrm{D}\mathcal{E}(q)) \equiv 0$, which implies the second relation in (1.2). Since $\mathcal{J}(q)\mathrm{D}\mathcal{S}(q) \equiv 0$ also holds we have a GENERIC system.

In particular, we consider the case that z describes a finite number of macroscopic heat baths, each of which is fully characterized by its temperature $\theta_m(t)$ and its fixed heat capacity $c_m > 0$, i.e. with $z = \theta := (\theta_1, ..., \theta_M) \in]0, \infty[^M$ we have

$$E(\theta) = c \cdot \theta = \sum_{m=1}^{M} c_m\theta_m \quad \text{and} \quad S(\theta) = \sum_{m=1}^{M} c_m \log \theta_m.$$

Note that $\mathcal{E}$ is a linear functional in $q = (\rho, \theta)$ while $\mathcal{S}$ is strictly concave. Thus, for each given energy level E_0 there is a unique maximizer of $\mathcal{S}$ subject to $\mathcal{E}(\rho, \theta) = E_0$ called the thermodynamic equilibrium, which is given as

$$q_{\mathbf{eq}} = (\rho_{\mathbf{eq}}, \theta_{\mathbf{eq}}) \quad \text{with } \theta_{\mathbf{eq}} = \theta_*(1, , ..., 1) \text{ and } \rho_{\mathbf{eq}} = \tfrac{1}{Z} \exp\Big(\frac{-1}{k_{\mathrm{B}}\theta_*} H\Big),$$

where Z and θ_* depend on E_0 only. By the abstract theory of GENERIC (cf. Section 2.2) this $q_{\mathbf{eq}}$ is an equilibrium independently of the choice of $\mathcal{J}$ and $\mathcal{K}$ if (1.2) holds.

To prove a global existence result for the associated evolutionary system (1.1) we further specify the dissipation by choosing the super-operators $\boldsymbol{C}_m$ suitably. We follow [Gra82, Ött10, Ött11] and use the inverse of the so-called Bogoliubov-Kubo-Mori metric (cf. [Str96, Str00, MPA00]) given by

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

We call $\mathcal{C}_\rho$ the ***canonical correlation operator*** and refer to the above references for the relevance of this metric. There is a strong relation between the von Neumann entropy and $\mathcal{C}_\rho$ encoded in the commutator relations

$$\big[\mathcal{C}_\rho A, \log \rho\big] = \big[A, \rho\big] = \mathcal{C}_\rho\big[A, \log \rho\big], \tag{1.3}$$

for all $A = A^*$ and $\rho \in \mathfrak{R}$. Recall that $\mathrm{D}_\rho \mathcal{S} = -k_{\mathrm{B}} \log \rho$ and note that $\mathrm{D}_\rho^2 \mathcal{S} = \mathcal{C}_\rho^{-1}$, see [MPA00]. A proof of (1.3) is given in Section 4.1, where also the continuity of the mapping $\mathfrak{R} \ni \rho \mapsto \mathcal{C}_\rho$ is established.

Choosing $\boldsymbol{C}_m = \mathcal{C}_\rho$ and $\alpha_j = \frac{1}{c_{m(j)}} \boldsymbol{e}_{m(j)} \in \mathbb{R}^M$ we arrive at the system

$$\dot\rho = \jmath[\rho, H] - \sum_{m=1}^{M} \sum_{n=1}^{N_m} \big[\, Q_m^n \,,\, k_{\mathrm{B}}[Q_m^n, \rho] + \frac{1}{\theta_m} \mathcal{C}_\rho[Q_m^n, H] \,\big], \tag{1.4a}$$

$$\dot\theta = \kappa\big(\tfrac{c_m}{\theta_m}\big)_{m=1,\dots,M} + \Big(\frac{1}{c_m} \sum_{n=1}^{N_m} \langle\!\langle\, k_{\mathrm{B}}[Q_m^n, \rho] + \tfrac{1}{\theta_m} \mathcal{C}_\rho[Q_m^n, H] \,\|\, [Q_m^n, H] \,\rangle\!\rangle\Big)_{m=1,..,M}, \tag{1.4b}$$

which will be discussed in Section 4. The equation for ρ displays dissipative double commutators $[Q, [Q, \rho]]$ of the Lindblad type in (1.4a) with a correction term involving the nonlinear term $\rho \mapsto [Q, \mathcal{C}_\rho[Q, H]]$. The latter term is continuous but not Lipschitz continuous on $\mathfrak{R}$. Moreover, we see a clear coupling to the temperatures θ_m in the different heat baths.

In Section 6 we discuss the isothermal case where the underlying Hilbert space $\boldsymbol{H}$ is finite-dimensional, i.e. $\boldsymbol{H} = \mathbb{C}^{\dim \boldsymbol{H}}$, which leads to the system

$$\dot\rho = \jmath[\rho, H] - \sum_{n=1}^{N} \big[Q^n, k_{\mathrm{B}}[Q^n, \rho] + \frac{1}{\theta_*} \mathcal{C}_\rho[Q^n, H]\big], \tag{1.5}$$

where now the temperature $\theta_* > 0$ is fixed. This is a dissipative Hamiltonian system of the form $\dot\rho = \big(J(\rho) - \frac{1}{\theta_*} K(\rho)\big) \mathrm{D}\mathcal{F}(\rho)$ for the free energy

$$\mathcal{F}(\rho) = \langle\!\langle\, \rho \,\|\, H \,\rangle\!\rangle + k_{\mathrm{B}}\theta_* \langle\!\langle\, \rho \,\|\, \log \rho \,\rangle\!\rangle.$$

Global existence of solutions is established in Theorem 6.2, and Theorem 6.4 provides conditions on the coupling operators Q^n such that all solutions satisfy $\rho(t) \to \rho_{\mathbf{eq}}$ for $t \to \infty$. In Section 5.3 we

discuss the case $\dim \boldsymbol{H} = 2$ in detail and display the dynamics in suitable coordinates as an ODE in $\mathbb{R}^3$.

The linear Lindblad systems (cf. [Lin83, Lin76, Gra82]) can be understood as approximations of (1.5) after replacing the super-operator $\mathcal{C}_\rho$ by the constant $\mathcal{C}_{\rho_{\mathsf{eq}}}$. Using (1.3) we have $\mathcal{C}_{\rho_{\mathsf{eq}}}[Q,H] = -k_{\mathrm{B}}\theta_*[Q,\rho_{\mathsf{eq}}]$ and arrive at (see Section 4.4),

$$\dot\rho = \jmath[\rho,H] - \sum_{n=1}^{N}\big[Q^n, k_{\mathrm{B}}[Q^n,\rho-\rho_{\mathsf{eq}}]\big] \quad \text{with } \rho_{\mathsf{eq}} = \frac{1}{Z}\exp\big(\frac{-1}{k_{\mathrm{B}}\theta_*}H\big). \tag{1.6}$$

Section 7 gives some analogies between the gradient structure $\dot\rho = \mathcal{K}^{\boldsymbol{Q}}(\rho)\mathrm{D}\mathcal{S}_{\mathrm{qm}}(\rho)$ used here and two other entropy gradient structures for stochastic problems, namely that for the Fokker-Planck equation introduced in [JKO98, Ott01] and that for reversible Markov chains introduced in [Maa11, Mie11b]. All structures have the common feature that the mapping $\rho \mapsto K(\rho)$ is homogeneous of degree 1, i.e. $K(\lambda\rho) = \lambda K(\rho)$. Moreover, K is defined in terms of couplings in the discrete case or derivatives relating to transportation in the continuous case.

2 The GENERIC framework

The framework of GENERIC was introduced by Öttinger and Grmela in [GrÖ97, ÖtG97]. It is based on a quintuple $(\mathcal{Q},\mathcal{E},\mathcal{S},\mathcal{J},\mathcal{K})$, 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 structure, namely a Poisson structure $\mathcal{J}$ and a dissipative structure $\mathcal{K}$, i.e., for each $q \in \mathcal{Q}$ the operators $\mathcal{J}(q)$ and $\mathcal{K}(q)$ 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 by the differential equation

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

where $\mathrm{D}\mathcal{E}$ and $\mathrm{D}\mathcal{S}$ are the differentials taking values in the cotangent space.

We refer to [GrÖ97, ÖtG97, Grm10] for applications in fluid mechanics, to [JHÖ06] for electromagnetism, to [Mie11a] for applications of GENERIC in elastoplastic materials. The book [Ött05] contains a general introduction with an emphasis towards numerical simulation. Subsequently we will mainly dwell on the quantum mechanical papers [Ött10, Ött11].

2.1 The structure of GENERIC

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

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

and the structural properties

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

Jacobi's identity for $\mathcal{J}$ means $\{\{\mathcal{F}_1,\mathcal{F}_2\}_{\mathcal{J}},\mathcal{F}_3\}_{\mathcal{J}} + \{\{\mathcal{F}_2,\mathcal{F}_3\}_{\mathcal{J}},\mathcal{F}_1\}_{\mathcal{J}} + \{\{\mathcal{F}_3,\mathcal{F}_1\}_{\mathcal{J}},\mathcal{F}_2\}_{\mathcal{J}} \equiv 0$ for all functions $\mathcal{F}_j : \mathcal{Q} \to \mathbb{R}$, where the Poisson bracket is defined via

$$\{\mathcal{F},\mathcal{G}\}_{\mathcal{J}}(q) := \langle \mathrm{D}\mathcal{F}(q), \mathcal{J}(q)\mathrm{D}\mathcal{G}(q)\rangle.$$

Finally, 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 (NIC)***:

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

Of course, the structure of GENERIC is geometric in the sense that it is invariant under coordinate transformations. Introducing new coordinates $q = x(Y)$ we define the transformed functionals $\overline{\mathcal{E}}$ and $\overline{\mathcal{S}}$ in the usual way, namely

$$\overline{\mathcal{E}}(Y) = \mathcal{E}(x(Y)) \text{ and } \overline{\mathcal{S}}(Y) = \mathcal{S}(x(Y)).$$

Moreover, the transformed geometric structures $\overline{\mathcal{J}}$ and $\overline{\mathcal{K}}$ are obtained via

$$\overline{\mathcal{J}}(Y) = \mathrm{D}x(Y)^{-1}\mathcal{J}(x(Y))\mathrm{D}x(Y)^{-*} \text{ and } \overline{\mathcal{K}}(Y) = \mathrm{D}x(Y)^{-1}\mathcal{K}(x(Y))\mathrm{D}x(Y)^{-*}, \tag{2.5}$$

where $\mathrm{D}x(Y)^{-*} : \mathrm{T}^*_Y\mathcal{Y} \to \mathrm{T}^*_{x(Y)}\mathcal{Q}$ denotes the adjoint of the inverse of $\mathrm{D}x(Y) : \mathrm{T}_Y\mathcal{Y} \to \mathrm{T}_{x(Y)}\mathcal{Q}$. Clearly, the transformed system $\dot{Y} = \overline{\mathcal{J}}(Y)\mathrm{D}\overline{\mathcal{E}}(Y) + \overline{\mathcal{K}}(Y)\mathrm{D}\overline{\mathcal{S}}(Y)$ is equivalent to the original system (2.1).

2.2 Properties of GENERIC systems

The first observation is that (2.3) and (2.4) imply energy conservation and entropy increase:

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(q(t)) = \langle \mathrm{D}\mathcal{S}(q), \dot{q}\rangle = \langle \mathrm{D}\mathcal{S}(q), \mathcal{J}\mathrm{D}\mathcal{E} + \mathcal{K}\mathrm{D}\mathcal{S}\rangle = 0 + \langle \mathrm{D}\mathcal{S}, \mathcal{K}\mathrm{D}\mathcal{S}\rangle \geq 0. \tag{2.7}$$

Note that we would need much less than the two conditions (2.3) and (2.4) to guarantee these two properties. However, the next property needs (2.4) in its full strength.

Next, we show that equilibria can be obtained by the ***maximum entropy principle***. If x_{eq} maximizes $\mathcal{S}$ under the constraint $\mathcal{E}(q) = E_0$, then we obtain a Lagrange multiplier $\lambda_{\mathrm{eq}} \in \mathbb{R}$ such that $\mathrm{D}\mathcal{S}(q_{\mathrm{eq}}) = \lambda_{\mathrm{eq}}\mathrm{D}\mathcal{E}(q_{\mathrm{eq}})$. Assuming that $\lambda_{\mathrm{eq}} \neq 0$ we immediately find that x_{eq} is an equilibrium of (2.1). Indeed,

$$\mathcal{J}(q_{\mathrm{eq}})\mathrm{D}\mathcal{E}(q_{\mathrm{eq}}) = \tfrac{1}{\lambda_{\mathrm{eq}}}\mathcal{J}(q_{\mathrm{eq}})\mathrm{D}\mathcal{S}(q_{\mathrm{eq}}) = 0 \text{ and } \mathcal{K}(q_{\mathrm{eq}})\mathrm{D}\mathcal{S}(q_{\mathrm{eq}}) = \lambda_{\mathrm{eq}}\mathcal{K}(q_{\mathrm{eq}})\mathrm{D}\mathcal{E}(q_{\mathrm{eq}}) = 0,$$

where we have used the NIC (2.4).

Vice versa, for every steady state q_{eq} of (2.1) we must have

$$\mathcal{J}(q_{\mathrm{eq}})\mathrm{D}\mathcal{E}(q_{\mathrm{eq}}) = 0 \text{ and } \mathcal{K}(q_{\mathrm{eq}})\mathrm{D}\mathcal{S}(q_{\mathrm{eq}}) = 0. \tag{2.8}$$

Thus, in a steady state there cannot be any balancing between reversible and irreversible forces, both have to vanish independently. To see this we simply recall the entropy production relation (2.7), which implies $\langle \mathrm{D}\mathcal{S}(q_{\mathrm{eq}}), \mathcal{K}(q_{\mathrm{eq}})\mathrm{D}\mathcal{S}(q_{\mathrm{eq}})\rangle$ for any steady state. Since $\mathcal{K}(q_{\mathrm{eq}})$ is positive semidefinite, this implies the second identity in (2.8). The first identity then follows from $\dot{q} \equiv 0$ in (2.1).

2.3 Isothermal systems

Often temperature effects can be neglected and the model can be approximated by an isothermal system. We show here how this can be deduced consistently from the GENERIC form if we add some coupling to an external heat bath fixed to a given temperature $\theta_* > 0$. In particular, we will replace the two functionals $\mathcal{E}$ and $\mathcal{S}$ by one, namely the free energy $\mathcal{F}_*$ at the given temperature θ_*.

We start from a general system for the variable $q = (y, \theta)$ in the form

$$\begin{pmatrix} \dot{y} \\ \dot{\theta} \end{pmatrix} = \begin{pmatrix} J & \alpha \\ -\alpha^{\mathsf{T}} & 0 \end{pmatrix} \begin{pmatrix} \mathrm{D}_y \overline{\mathcal{E}} \\ \mathrm{D}_\theta \overline{\mathcal{E}} \end{pmatrix} + \begin{pmatrix} K & \beta \\ \beta^{\mathsf{T}} & \Lambda \end{pmatrix} \begin{pmatrix} \mathrm{D}_y \overline{\mathcal{S}} \\ \mathrm{D}_\theta \overline{\mathcal{S}} \end{pmatrix} - \begin{pmatrix} 0 \\ A(\theta - \theta_*) \end{pmatrix}, \tag{2.9}$$

where the coupling operator A is assumed to be positive definite. Defining the functional $\mathcal{F}^\circ(y, \theta) = \overline{\mathcal{E}}(y, \theta) - \theta_* \overline{\mathcal{S}}(y, \theta)$, the system (2.9) takes the form

$$\begin{pmatrix} \dot{y} \\ \dot{\theta} \end{pmatrix} = \begin{pmatrix} J - \frac{1}{\theta_*} K & \alpha - \frac{1}{\theta_*} \beta \\ -\alpha^{\mathsf{T}} - \frac{1}{\theta_*} \beta^{\mathsf{T}} & -\frac{1}{\theta_*} \Lambda \end{pmatrix} \begin{pmatrix} \mathrm{D}_y \mathcal{F}^\circ \\ \mathrm{D}_\theta \mathcal{F}^\circ \end{pmatrix} - \begin{pmatrix} 0 \\ A(\theta - \theta_*) \end{pmatrix}.$$

The equation for $\dot{y}$ reads $\dot{y} = \big(J - \frac{1}{\theta_*} K\big) \mathrm{D}\mathcal{F}^\circ + \big(\alpha - \frac{1}{\theta_*} \beta\big) \mathrm{D}_\theta \mathcal{F}^\circ$, where the last term vanishes to order $O(\|\theta - \theta_*\|)$, see [Mie11a, Sect. 2.6] for more details. Defining the isothermal free energy $\mathcal{F}_*(y) = \mathcal{F}^\circ(y, \theta_*)$ and neglecting all terms of order $O(\theta - \theta_*)$ we arrive at the isothermal damped Hamiltonian system

$$\dot{y} = \big(J(y, \theta_*) - \frac{1}{\theta_*} K(y, \theta_*)\big) \mathrm{D}\mathcal{F}_*(y). \tag{2.10}$$

Note that J still defines a Poisson structure and that K is positive semi-definite. Hence, $\mathcal{F}_*$ is a Liapunov function for (2.10).

3 Coupling of quantum and dissipative mechanics

3.1 Quantum mechanics

The quantum mechanical system is described by states in a 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 Schrödinger equation

$$\dot{\psi} = -\jmath H \psi, \quad \text{where } \jmath = \frac{\mathrm{i}}{\hbar}, \tag{3.1}$$

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, such that

$$\|A\|_p := \Big(\sum_{j=1}^{\infty} \sigma_j(A)^p \Big)^{1/p} < \infty,$$

where σ_j is the jth singular value of A (i.e. the jth largest eigenvalue of $(A^*A)^{1/2}$). We refer to [GoK69, Ch. III] for this and the following standard properties. Moreover, $\mathcal{L}^\infty(\boldsymbol{H})$ is the set of bounded linear operators with $\|A\|_\infty$ denoting the standard operator norm. For $1 \le p_1 < p_2 < \infty$ we have

$$\mathcal{L}^{p_1}(\boldsymbol{H}) \subset \mathcal{L}^{p_2}(\boldsymbol{H}) \text{ and } \|A\|_{p_1} \ge \|A\|_{p_2} \text{ for all } A \in \mathcal{L}^{p_1}(\boldsymbol{H}).$$

Moreover, if $1/p = 1/p_1 + 1/p_2 \le 1$, then Hölder's estimate holds

$$\|AB\|_q \le \|A\|_{p_1}\|B\|_{p_2} \text{ for all } A \in \mathcal{L}^{p_1}(\boldsymbol{H}),\ B \in \mathcal{L}^{p_2}(\boldsymbol{H}). \tag{3.2}$$

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 and $\mathcal{L}^p(\boldsymbol{H})' \cong \mathcal{L}^q(\boldsymbol{H})$ for $1 < p, q < \infty$ with $1/p + 1/q = 1$. We will need the following elementary commutator relations:

$$\begin{aligned} &\langle\!\langle\, A \,\|\, BC \,\rangle\!\rangle = \langle\!\langle\, B^*A \,\|\, C \,\rangle\!\rangle = \langle\!\langle\, AC^* \,\|\, B \,\rangle\!\rangle, \text{ giving} \\ &\langle\!\langle\, A \,\|\, [B,C] \,\rangle\!\rangle = \langle\!\langle\, [B^*,A] \,\|\, C \,\rangle\!\rangle = -\langle\!\langle\, [A,B^*] \,\|\, C \,\rangle\!\rangle = \langle\!\langle\, [A,C^*] \,\|\, B \,\rangle\!\rangle. \end{aligned} \tag{3.3}$$

To couple a quantum system to a macroscopic one we need to describe it in terms of the multi-particle form using the density matrices

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

Hence, each $\rho \in \mathfrak{R}$ has the representation

$$\rho = \sum_{j=1}^\infty r_j\, \psi_j \otimes \overline{\psi}_j, \tag{3.4}$$

where $r_j \ge 0$, $\sum_1^\infty r_j = 1$, and $\{\,\psi_j \,|\, j \in \mathbb{N}\,\}$ is an orthonormal set. (Note that $(\psi \otimes \overline{\phi})a := \langle a|\phi\rangle\psi$ and $(\psi \otimes \overline{\phi})A = \psi \otimes \overline{A}^*\phi$.) Using (3.1) the evolution of ρ is given via the Liouville equation

$$\dot\rho = \jmath[\rho, H], \quad \text{where } [\rho, H] := \rho H - H\rho. \tag{3.5}$$

This is consistent with (3.1) if each of the ψ_j solves (3.1) while all r_j are constant.

Below we will use the von Neumann entropy

$$S_{\mathrm{qm}}(\rho) = -k_{\mathrm{B}}\langle\!\langle\, \rho \,\|\, \log\rho \,\rangle\!\rangle = -k_{\mathrm{B}}\,\mathrm{tr}(\rho\log\rho) = -k_{\mathrm{B}}\sum_{j=1}^\infty r_j \log r_j. \tag{3.6}$$

It is easy to see that the entropy remains constant in the Hamiltonian case.

While the single-commutator equation (3.5) gives rise to Hamiltonian dynamics, the following double-commutator equation leads to dissipative dynamics:

$$\dot\eta = -[Q,[Q,\eta]] = -(Q^2\eta - 2Q\eta Q + \eta Q^2), \tag{3.7}$$

where $Q \in \mathcal{L}^p_{\mathrm{S}}(\boldsymbol{H})$ is a given operator. As Q can be written in the form $\sum_{n=1}^{\infty} q_n \phi_n \otimes \overline{\phi}_n$ we easily find that the corresponding coefficients $\eta_{nm}(t) = \langle \rho(t)\phi_n | \phi_m \rangle$ satisfy the ODE

$$\dot{\eta}_{nm} = -(q_n - q_m)^2 \eta_{nm}.$$

Thus, the double-commutator evolution diminishes all off-diagonal elements, while the diagonal elements of η (and hence the trace) remain unchanged. Hence, a typical dissipative quantum system is Lindblad equation of the form

$$\dot{\rho} = \jmath[\rho, H] - \sum_{n=1}^{N} \big[Q^n, [Q^n, \rho - \rho_{\mathbf{eq}}]\big]. \tag{3.8}$$

While it is well-known that this equation preserves the property that $\rho(t) \in \mathfrak{R}$ it is less clear what the longtime dynamics is and what suitable Liapunov function are. We will see later that the GENERIC framework leads to a correction of (3.8), see Section 4.4.

3.2 Dissipative evolution

We assume that an additional variable z is present in the model that is dissipative. For simplicity, we assume that z lies in a closed subset $Z \subset \boldsymbol{Z} = \mathbb{R}^N$. The evolution is assumed to be purely dissipative in the sense that it is a gradient flow with respect to the entropy $S : Z \to \mathbb{R}$, namely

$$\dot{z} = K(z)\mathrm{D}S(z), \text{ where } K(z) = K(z)^{\mathsf{T}} \geq 0. \tag{3.9}$$

We immediately obtain entropy production in the form

$$\frac{\mathrm{d}}{\mathrm{d}t} S(z(t)) = \mathrm{D}S(z) \cdot K(z)\mathrm{D}S(z) \geq 0.$$

If an energy $E : Z \to \mathbb{R}$ is conserved along solutions z of (3.9), then the relation $\mathrm{D}E(z) \cdot K(z)\mathrm{D}S(z) \equiv 0$ has to hold. Very often one imposes the stronger condition

$$K(z)\mathrm{D}E(z) \equiv 0,$$

which is certainly sufficient, but not at all necessary.

3.3 Coupling of the models

We now couple the quantum and the dissipative system in the GENERIC sense. The joint state space is $\mathcal{Q} = \mathfrak{R} \times Z \subset \mathcal{L}^1_{\mathrm{S}}(\boldsymbol{H}) \times \mathbb{R}^N$, where the state is given by the pair (ρ, z). The energy functional $\mathcal{E}$ and the entropy functional $\mathcal{S}$ take the form

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

In the general case, the Hamiltonian H may depend on the dissipative variable z, but for our mathematical results we assume that H is independent of z. For the Poisson structure we assume that the variable z is totally dissipative, which means that $\mathcal{J}$ has block structure on the form

$$\mathcal{J}(\rho, z) = \begin{pmatrix} \jmath[\rho, \square\,] & 0 \\ 0 & 0 \end{pmatrix},$$

where $\square$ indicates, where the corresponding component of the vector applied from the right has to be inserted. The dissipation operator is first defined in terms of the dissipation potential, which is quadratic in the driving forces

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

In the following we use a special ansatz for the dissipation potential that is based on the physical observation that a quantum mechanical system interacts with its environment only via the commutators with respect to suitable coupling operators $Q_m(z) \in \mathcal{L}^\infty_\mathrm{S}(\boldsymbol{H})$. This leads to

$$\Big\langle \mathcal{K}(\rho,z)\begin{pmatrix}\mu\\ \zeta\end{pmatrix}\Big|\begin{pmatrix}\mu\\ \zeta\end{pmatrix}\Big\rangle = \zeta\cdot K_\mathsf{diss}(\rho,z)\zeta + \sum_{m=1}^M \|\!|[Q_m(z),\mu-\alpha_m(\rho,z)\cdot\zeta\, H(z)]|\!\|^2_{\boldsymbol{C}_m(\rho,z)},$$

where $\alpha_m(\rho,z)\in\mathbb{R}^N$, $K_\mathsf{diss}(\rho,z)\in\mathbb{R}^{N\times N}$ is symmetric and positive semidefinite, and the super-operators $\boldsymbol{C}_m(\rho,z)$ are symmetric and positive semidefinite on $\mathcal{L}^2(\boldsymbol{H})$. (Here super-operators are linear operator on $\mathcal{L}^p(\boldsymbol{H})$.) The norm $\|\!|\cdot|\!\|_{\boldsymbol{C}}$ is defined via

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

To simplify the following notations we introduce another super-operator

$$\mathcal{K}^Q_{\boldsymbol{C}} : A \mapsto [Q^*,\boldsymbol{C}[Q,A]].$$

Using (3.3) the associated linear operator K takes the form

$$\mathcal{K}(q) = \begin{pmatrix}0 & 0\\ 0 & K_\mathsf{diss}\end{pmatrix} + \sum_{m=1}^M \begin{pmatrix}\mathcal{K}^{Q_m}_{\boldsymbol{C}_m} & -(\alpha_m\cdot\square)\,\mathcal{K}^{Q_m}_{\boldsymbol{C}_m}H\\ -\langle\!\langle\, \mathcal{K}^{Q_m}_{\boldsymbol{C}_m}\square \,\|\, H\,\rangle\!\rangle\alpha_m & \langle\!\langle\, \mathcal{K}^{Q_m}_{\boldsymbol{C}_m}H \,\|\, H\,\rangle\!\rangle\alpha_m\otimes\overline{\alpha}_m\end{pmatrix},$$

where we have omitted the arguments ρ and z for simplicity. The occurrence of double commutators $\mathcal{K}^{Q_m}_{\boldsymbol{C}_m}$ indicates the dissipative nature of K.

To satisfy the NIC (2.4) we still need an assumption on $\mathcal{K}$, namely

$$K_\mathsf{diss}(\rho,z)\mathrm{D}_z\mathcal{E}(\rho,z)) = 0 \text{ and } \alpha_m(\rho,z)\cdot\mathrm{D}_z\mathcal{E}(\rho,z)) = 1 \quad \text{for all } m,\rho,z. \tag{3.10}$$

These assumptions guarantee $\mathcal{K}(q)\mathrm{D}\mathcal{E}(q)\equiv 0$. Thus, $\mathcal{J}(\rho,z)$ and the symmetric and positive linear operator $\mathcal{K}$ satisfy the NIC (2.4), i.e. $\mathcal{J}(\rho,z)\mathrm{D}\mathcal{S}(\rho,z)\equiv 0$ and $\mathcal{K}(\rho,z)\mathrm{D}\mathcal{E}(\rho,z)\equiv 0$. Now the GENERIC formalism provides the evolutionary system for $q=(\rho,z)$, namely

$$\begin{aligned}
\dot\rho &= \jmath[H(z),\rho] - \sum_1^M \mathcal{K}^{Q_m(z)}_{\boldsymbol{C}_m(\rho,z)}\Big(k_\mathrm{B}\log\rho+\alpha_m(\rho,z)\cdot\mathrm{D}S(z)H(z)\Big),\\
\dot z &= K_\mathsf{diss}(\rho,z)\mathrm{D}S(z)+\\
&\quad + \sum_1^M \langle\!\langle\, \mathcal{K}^{Q_m(z)}_{\boldsymbol{C}_m(\rho,z)}\big(k_\mathrm{B}\log\rho+\alpha_m(\rho,z)\cdot\mathrm{D}S(z)H(z)\big) \,\|\, H(z)\,\rangle\!\rangle\alpha_m(\rho,z).
\end{aligned} \tag{3.11}$$

In the following we will reduce the generality in order to obtain more structure.

4 Canonical correlation

4.1 The Kubo-Mori metric

Following [Gra82, Ött11] we introduce a ***canonical correlation operator*** which associates with the density matrix ρ in the following way: for each $\rho \in \mathfrak{R}$ we define

$$\mathcal{C}_\rho : \left\{ \begin{array}{ccc} \mathcal{L}^\infty(\boldsymbol{H}) & \to & \mathcal{L}^1(\boldsymbol{H}), \\ A & \mapsto & \int_0^1 \rho^s A \rho^{1-s} \, \mathrm{d}s. \end{array} \right. \tag{4.1}$$

The boundedness follows from Hölder's estimate (3.2) giving

$$\|\mathcal{C}_\rho A\|_q \leq \|\rho\|_{p_1} \|A\|_{p_2} \quad \text{for } \frac{1}{q} = \frac{1}{p_1} + \frac{1}{p_2}.$$

We further have the identity $(\mathcal{C}_\rho A)^* = \mathcal{C}_\rho(A^*)$ (using reparametrization and $\rho = \rho^*$). If ρ has the representation $\sum r_j \psi_j \otimes \overline{\psi}_j$, then we have

$$\mathcal{C}_\rho A = \sum_{j,k=1}^{\dim \boldsymbol{H}} \Lambda(r_j, r_k) \langle A\psi_k | \psi_j \rangle \psi_j \otimes \overline{\psi}_k \text{ and } \langle\!\langle \, \mathcal{C}_\rho A \, \| \, A \, \rangle\!\rangle = \sum_{j,k=1}^{\dim \boldsymbol{H}} \Lambda(r_j, r_k) \big| \langle A\psi_k | \psi_j \rangle \big|^2, \tag{4.2}$$

where the continuous function $\Lambda : [0, \infty[^2 \to [0, \infty[$ is given by

$$\Lambda(a,b) = \int_0^1 a^s b^{1-s} \, \mathrm{d}s = \left\{ \begin{array}{ll} \frac{a-b}{\log a - \log b} & \text{for } a, b > 0 \text{ and } a \neq b, \\ a & \text{for } a = b \geq 0, \\ 0 & \text{for } \min\{a,b\} = 0. \end{array} \right. \tag{4.3}$$

Note that Λ satisfies the bounds $\min\{a,b\} \leq \sqrt{ab} \leq \Lambda(a,b) \leq \frac{1}{2}(a+b) \leq \max\{a,b\}$.

Thus, we have on $\mathcal{L}^\infty(\boldsymbol{H})$ the relations

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

which induce the scalar product $(A, B) \mapsto \langle\!\langle \, \mathcal{C}_\rho A \, \| \, B \, \rangle\!\rangle$. This scalar product 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

$$\mathcal{G}_\rho A := \mathcal{C}_\rho^{-1} A = \int_0^\infty (\rho + sI)^{-1} A (\rho + sI)^{-1} \, \mathrm{d}s. \tag{4.4}$$

This formula is most easily derived from (4.2) by using $1/\Lambda(a,b) = \int_0^\infty \big((a+s)(b+s)\big)^{-1} \, \mathrm{d}s$. The tensor $\mathcal{G}_\rho$ defines the ***Bogoliubov-Kubo-Mori metric*** on the set of density matrices as follows, see [Pet94, PeS99, MPA00]. For a curve $[0,1] \ni s \mapsto \widetilde{\rho}(s)$ we define its Kubo-Mori length $\ell(\widetilde{\rho})$ via

$$\ell(\widetilde{\rho})^2 = \int_0^1 \langle\!\langle \, \widetilde{\rho}'(s) \, \| \, \mathcal{G}_{\widetilde{\rho}(s)} \widetilde{\rho}'(s) \, \rangle\!\rangle \, \mathrm{d}s.$$

The relevance of the Bogoliubov-Kubo-Mori metric as a generalization of the Fisher information metric is discussed in the above references. For our usage, the most important fact is the connection to the von Neumann entropy S_{qm}, see (3.6). In fact, $\mathcal{G}_\rho$ can be identified by its Hessian, namely

$$\langle\!\langle \, A \, \| \, \mathrm{D}^2 S_{\mathrm{qm}}(\rho) B \, \rangle\!\rangle = -k_{\mathrm{B}} \langle\!\langle \, A \, \| \, \mathcal{G}_\rho B \, \rangle\!\rangle.$$

Open problem 1: *Is the mapping $\mathfrak{R} \ni \rho \mapsto \langle\!\langle\, A \,\|\, \mathcal{C}_\rho A \,\rangle\!\rangle$ concave for all A? A positive answer would give good metric properties for the Riemannian manifold $(\mathfrak{R}, \mathcal{G}_\rho)$, see [LiM12].*

The following identities, 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 $S_{\rm qm}$ and the canonical correlation operator $\mathcal{C}_\rho$.

Proposition 4.1 *For all $A \in \mathcal{L}^\infty_{\rm S}(\boldsymbol{H})$ and all $\rho \in \mathfrak{R}$ with $\log \rho \in \mathcal{L}^\infty_{\rm S}(\boldsymbol{H})$ we have*

$$\big[\mathcal{C}_\rho A, \log \rho\big] = \big[A, \rho\big] = \mathcal{C}_\rho\big[A, \log \rho\big]. \tag{4.5}$$

Proof: For the convenience of the reader we give a full proof. With $P = \log \rho$ we have $\rho = \mathrm{e}^P$ and

$$\begin{aligned}\big[\mathcal{C}_\rho A, \log \rho\big] &= \int_0^1 \big[\mathrm{e}^{sP} A \mathrm{e}^{(1-s)P}, P\big]\,\mathrm{d}s = \int_0^1 \mathrm{e}^{sP} A(\mathrm{e}^{(1-s)P} P) - (P\mathrm{e}^{sP}) A \mathrm{e}^{(1-s)P}\,\mathrm{d}s \\ &= \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}\big(-\mathrm{e}^{sP} A \mathrm{e}^{(1-s)P}\big)\,\mathrm{d}s = -\big(\mathrm{e}^{sP} A \mathrm{e}^{(1-s)P}\big)_0^1 = \big[A, \mathrm{e}^P\big] = \big[A, \rho\big].\end{aligned}$$

With slightly different grouping, we also obtain the second identity, namely

$$\begin{aligned}\mathcal{C}_\rho\big[A, \log \rho\big] &= \int_0^1 \mathrm{e}^{sP}(AP - PA)\mathrm{e}^{(1-s)P}\,\mathrm{d}s = \int_0^1 \mathrm{e}^{sP} A(P\mathrm{e}^{(1-s)P}) - (\mathrm{e}^{sP} P) A \mathrm{e}^{(1-s)P}\,\mathrm{d}s \\ &= \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}\big(-\mathrm{e}^{sP} A \mathrm{e}^{(1-s)P}\big)\,\mathrm{d}s = \ldots = \big[A, \rho\big].\end{aligned}$$

Thus, both identities are established. ∎

The following result shows that $\mathcal{C}_\rho \in \mathrm{Lin}(\mathrm{L}^\infty_{\rm S}(\boldsymbol{H}), \mathrm{L}^1_{\rm S}(\boldsymbol{H}))$ depends continuously on $\rho \in \mathfrak{R} \in \mathrm{L}^1_{\rm S}(\boldsymbol{H})$ with respect to the norm topology. This result will be crucial for our existence theory. This property is derived from Phillips' result on Hölder continuity for $\rho \mapsto \rho^s$ in the appropriate norms.

Proposition 4.2 *For all $\rho_1, \rho_2 \in \mathrm{L}^1_{\rm S}(\boldsymbol{H})$ with $\rho_1, \rho_2 \geq 0$ and all $A \in \mathrm{L}^\infty_{\rm S}(\boldsymbol{H})$ we have*

$$\|C_{\rho_1} A - C_{\rho_2} A\|_1 \leq \omega\left(\frac{\|\rho_1 - \rho_2\|_1}{\|\rho_1\|_1 + \|\rho_2\|_1}\right)\big(\|\rho_1\|_1 + \|\rho_2\|_1\big)\|A\|_\infty, \tag{4.6}$$

where $\omega(\nu) = 2\frac{1-\nu}{|\log \nu|}$.

Proof: The proof relies on Phillips' inequality (see [BhH88, Thm. 4]):

$$X = X^* \geq Y = Y^* \geq 0 \text{ and } p \geq 1 \quad \Longrightarrow \quad \|X^{1/p} - Y^{1/p}\|_p \leq \|X - Y\|_1^{1/p}. \tag{4.7}$$

We need the result a for the two non-ordered operators ρ_1 and ρ_2. For this we define $V = \rho_2 - \rho_1$ and decompose it into its positive and negative parts, namely $V = V_+ - V_-$ with $V_+, V_- \geq 0$. With $Z := \rho_1 + V_+$ we have

$$Z = \rho_1 + V_+ \geq \rho_1 \geq 0 \quad \text{and} \quad Z = \rho_2 + V_- \geq \rho_2 \geq 0.$$

Applying Phillips' inequality (4.7) to these two ordered pairs we obtain

$$\|Z^{1/p}-\rho_1^{1/p}\|_p \le \|Z-\rho_1\|_1^{1/p} = \|V_+\|_1^{1/p} \text{ and } \|Z^{1/p}-\rho_2^{1/p}\|_p \le \|Z-\rho_2\|_1^{1/p} = \|V_-\|_1^{1/p}.$$

Thus, the triangle estimate gives the desired generalization of (4.7), namely

$$\|\rho_2^{1/p}-\rho_1^{1/p}\|_p \le \|V_+\|_1^{1/p} + \|V_-\|_1^{1/p} \le 2^{1-1/p}\|V\|_1^{1/p} = 2^{1-1/p}\|\rho_1-\rho_2\|_1^{1/p}, \tag{4.8}$$

where we have used $\|V_+\|_1 + \|V_-\|_1 = \|V\|_1$ and

$$\alpha^{1/p}+\beta^{1/p} \le 2^{1-1/p}(\alpha+\beta)^{1/p} \text{ for all } p\ge 1,\ \alpha,\beta\ge 0. \tag{4.9}$$

We now estimate $C_{\rho_1}A - C_{\rho_2}A$ in $\mathrm{L}^1_{\mathrm{S}}(\boldsymbol{H})$ as follows:

$$\begin{aligned}
\|C_{\rho_1}A-C_{\rho_2}A\|_1 &\le \int_{s=0}^1 \|\rho_1^s A\rho_1^{1-s}-\rho_2^s A\rho_1^{1-s}\|_1 + \|\rho_2^s A\rho_1^{1-s}-\rho_2^s A\rho_2^{1-s}\|_1\,\mathrm{d}s\\
&\le \int_{s=0}^1 \|\rho_1^s-\rho_2^s\|_{1/s}\|A\|_\infty\|\rho_1^{1-s}\|_{1/(1-s)} + \|\rho_2^s\|_{1/s}\|A\|_\infty\|\rho_1^{1-s}-\rho_2^{1-s}\|_{1/(1-s)}\,\mathrm{d}s\\
&\le \|A\|_\infty \int_{r=0}^1 \|\rho_1^r-\rho_2^r\|_{1/r}\big(\|\rho_1\|_1^{1-r}+\|\rho_2\|_1^{1-r}\big)\,\mathrm{d}r\\
&\le \|A\|_\infty \int_{r=0}^1 2^{1-r}\|\rho_1-\rho_2\|_1^r\, 2^{1-(1-r)}\big(\|\rho_1\|_1+\|\rho_2\|_1\big)^{1-r}\,\mathrm{d}r,
\end{aligned}$$

where we have used (4.8) and (4.9) for the last estimate. Calculating the integral in the last expression gives the desired estimate (4.6). ∎

We emphasize that $\mathfrak{R}\ni\rho\mapsto\mathcal{C}_\rho\in\mathrm{Lin}(\mathrm{L}^\infty_{\mathrm{S}}(\boldsymbol{H}),\mathrm{L}^1_{\mathrm{S}}(\boldsymbol{H}))$, if $\mathfrak{R}$ is equipped with the norm of $\mathrm{L}^1_{\mathrm{S}}(\boldsymbol{H})$. Moreover, assuming $\dim\boldsymbol{H}<\infty$ and writing $\operatorname{int}\mathfrak{R}=\{\,\rho\mid\rho>0\,\}$ we see that $\operatorname{int}\mathfrak{R}\ni\rho\mapsto\mathcal{C}_\rho$ is an analytic function. For this we use that $R=\log\rho$ is an analytic function on $\operatorname{int}\mathfrak{R}$ and that $\mathcal{C}_\rho A=\int_0^1 \mathrm{e}^{sR}A\mathrm{e}^{(1-s)R}\,\mathrm{d}s$.

4.2 GENERIC systems with canonical correlation

We now specialize the general system (3.11) by choosing all the operators $\boldsymbol{C}_m$ equal to $\mathcal{C}_\rho$, as suggested in [Ött11]. However, we note that the dissipative bracket in [Ött11, Eqn. (10)] does not have the form assumed here. The point is now that the interaction of $\mathcal{C}_\rho$ with $\log\rho$ simplifies the evolutionary system considerably by invoking (4.5) giving

$$\mathcal{K}^Q_{\mathcal{C}_\rho}\log\rho = \big[Q,[Q,\rho]\big],$$

where the right-hand side is continuous, in contrast to $\log\rho$. We arrive at the system

$$\begin{aligned}
\dot\rho &= \jmath\big[H(z),\rho\big] - \sum_1^M \Big(k_{\mathrm{B}}\big[Q_m(z),[Q_m(z),\rho]\big] + \alpha_m(\rho,z)\cdot\mathrm{D}S(z)\mathcal{K}^{Q_m(z)}_{\mathcal{C}_\rho}H(z)\Big),\\
\dot z &= K_{\mathsf{diss}}(\rho,z)\mathrm{D}S(z)\\
&\quad + \sum_1^M \langle\!\langle\, k_{\mathrm{B}}\big[Q_m(z),[Q_m(z),\rho]\big] + \alpha_m(\rho,z)\cdot\mathrm{D}S(z)\mathcal{K}^{Q_m(z)}_{\mathcal{C}_\rho}H(z)\parallel H(z)\,\rangle\!\rangle\alpha_m(\rho,z).
\end{aligned}\tag{4.10}$$

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 (3.11).

We simplify the above system even further by assuming that it consists of M heat baths with temperatures $\theta = (\theta_1, \dots, \theta_M)$ and heat capacities $c_1, \dots, c_M > 0$. Each heat bath can interact with the quantum system by a finite number of coupling operators Q_m^n, $n = 1, ..., N_M$, which are independent of θ. Writing shortly $c = (c_m)$ we have the following GENERIC system $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathcal{J}, \mathcal{K})$ with

$$\mathcal{Q} = \mathfrak{R} \times]0,\infty[^M\,, \quad q = (\rho, \theta), \tag{4.11a}$$

$$\mathcal{E}(q) = \operatorname{tr}(\rho H) + c\cdot\theta, \quad \mathcal{S}(q) = -k_{\mathrm{B}}\operatorname{tr}(\rho\log\rho) + \textstyle\sum_{m=1}^M c_m \log\theta_m, \tag{4.11b}$$

$$\mathcal{J}(q) = \begin{pmatrix} \jmath[\rho, \square] & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathcal{K}(q) = \mathrm{D}^2\Psi^*_{(\xi,\tau)}(q;\xi,\tau), \tag{4.11c}$$

where the dual dissipation potential Ψ^* is given by

$$\Psi^*(\rho,\theta;\xi,\tau) = \tfrac{1}{2}\textstyle\sum_{m=1}^M \sum_{n=1}^{N_m} \|\!|[Q_m^n, \xi - \frac{\tau_m}{c_m}H]|\!\|^2_{\boldsymbol{C}_\rho} + \frac{1}{2}\tau\cdot\kappa\tau,$$

where $\kappa \in \mathbb{R}^{M\times M}_{\mathsf{sym}}$ is positive semidefinite with $\operatorname{kernel}\kappa = \operatorname{span} c$. A typical choice for κ is given by $\tau\cdot\kappa\tau = \sum_{m=1}^{M-1}\sum_{l=m+1}^{M}\kappa_{ml}\big(\frac{\tau_m}{c_m} - \frac{\tau_l}{c_l}\big)^2$, where the positive coefficients κ_{ml} give the direct heat transfer between the heat baths m and l. We have the NIC (2.4) because (i) $\mathrm{D}\mathcal{E}(q) = (H, c)$ and $\Psi^*(q;(H,c)) \equiv 0$ imply $\mathcal{K}(q)\mathrm{D}\mathcal{E}(q) \equiv 0$ and (ii) $\mathrm{D}\mathcal{S}(q) = (-k_{\mathrm{B}}\log\rho, *)$ implies $\mathcal{J}(q)\mathrm{D}\mathcal{S}(q) \equiv 0$.

The differential equation generated by the GENERIC system $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, \mathcal{J}, \mathcal{K})$ is

$$\dot\rho = \jmath[\rho, H] - \sum_{m=1}^M\sum_{n=1}^{N_m}\big[\, Q_m^n\,,\, k_{\mathrm{B}}[Q_m^n,\rho] + \frac{1}{\theta_m}\mathcal{C}_\rho[Q_m^n, H]\,\big], \tag{4.12a}$$

$$\dot\theta = \kappa\big(\tfrac{c_m}{\theta_m}\big)_{m=1,\dots,M} + \Big(\frac{1}{c_m}\sum_{n=1}^{N_m}\langle\!\langle\, k_{\mathrm{B}}[Q_m^n,\rho] + \tfrac{1}{\theta_m}\mathcal{C}_\rho[Q_m^n,H] \,\|\, [Q_m^n, H]\,\rangle\!\rangle\Big)_{m=1,..,M}. \tag{4.12b}$$

We nicely see the correction terms $\frac{1}{\theta_m}\big[Q_m^n, \mathcal{C}_\rho[Q_m^n, H]\big]$ to the otherwise linear Lindblad system $\dot\rho = \jmath[\rho,H] - k_{\mathrm{B}}\sum_{m=1}^M\sum_{n=1}^{N_m}\big[Q_m^n,[Q_m^n,\rho]\big]$.

If $\dim \boldsymbol{H} < \infty$ the right-hand side of (4.12) 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. In [MiN12] the global existence of solutions for (4.12) will be established. The difficulties arise if solutions reach the boundary of $\mathcal{Q}$, where the extension is nontrivial and may be nonunique. In Section 6 we only discuss an existence result for the simplified model presented in Section 5.

4.3 Steady states

We finally discuss the steady states for (4.12). By strict convexity of $\mathcal{S}$ there is a unique maximizer $q_{\mathsf{eq}} = (\rho_{\mathsf{eq}}, \theta_{\mathsf{eq}}) \in \mathcal{Q}$ subject to the constraint $\mathcal{E}(q) = E_0$, as soon as $E_0 > \lambda_{\mathsf{min}}(H)$. The latter condition is needed to make the admissible set $\{\, q \in \mathcal{Q} \mid \mathcal{E}(q) = E_0\,\}$ nonempty. The unique maximizer takes the form

$$\theta_{\mathsf{eq}}(E_0) = \theta_*(E_0)(1,...,1) \quad\text{and}\quad \rho_{\mathsf{eq}} = \frac{1}{Z(E_0)}\exp\big(\frac{-1}{k_{\mathrm{B}}\theta_*(E_0)}H\big). \tag{4.13}$$

By Section 2.2 we know that all $q_{\mathrm{eq}}(E_0)$ are steady states of (4.12).

The following result provides conditions showing that the family $q_{\mathrm{eq}}(E_0)$ provides the only steady states $q = (\rho, \theta)$ of (4.12) satisfying $\rho > 0$.

Theorem 4.3 *Assume* $\operatorname{kernel} \kappa = \operatorname{span} c$ *and that* $(Q_m^n)_{\substack{m=1,\dots,M \\ n=1,\dots,N_m}}$ *and* H *satisfy:*

$$\begin{aligned} &\textit{If } A = A^* \in \mathrm{Lin}(\boldsymbol{H}),\ [H, A] = 0, \textit{ and} \\ &\forall\, m = 1, ..., M\ \forall\, n = 1, ..., N_m: \quad [Q_m^n, A] = 0, \\ &\textit{then } A = \alpha I \textit{ for some } \alpha \in \mathbb{R}. \end{aligned} \tag{4.14}$$

Then, all steady states $q = (\rho, \theta) \in \mathcal{Q}$ *of* (4.12) *satisfying* $\rho > 0$ *have the form* $q_{\mathrm{eq}}(E_0)$ *for some* $E_0 \in \mathbb{R}$.

Proof: If q is a steady state with $q = (\rho, \theta)$ with $\rho > 0$, then $2\Psi^*(q, \mathrm{D}\mathcal{S}(q)) = \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(q) = 0$. Hence, we have

$$0 = \kappa \mathrm{D}_\theta \mathcal{S}(q) = \kappa\big(\tfrac{c_m}{\theta_m}\big)_{m=1,\dots,M}, \quad 0 = \|[Q_m^n, -k_{\mathrm{B}} \log \rho - \tfrac{1}{\theta_m} H]\|_{\mathcal{C}_\rho}.$$

Using $\operatorname{kernel} \kappa = \operatorname{span} c$ we obtain $\theta = (\theta_0, ..., \theta_0)$. Since $\rho > 0$ we have $\|A\|_{\mathcal{C}_\rho} = 0$ if and only if $A = 0$, whence

$$\forall\, m = 1, ..., M\ \forall\, n = 1, ..., N_m: \quad [Q_m^n, k_{\mathrm{B}} \log \rho + \tfrac{1}{\theta_0} H] = 0.$$

Inserting this into (4.12a) with $\dot\rho = 0$ (for a steady state) we also find $[\rho, H] = 0$. The latter implies $[H, k_{\mathrm{B}} \log \rho + \frac{1}{\theta_0} H]$, and we can apply (4.14) to $A = k_{\mathrm{B}} \log \rho + \frac{1}{\theta_0} H$. Now $k_{\mathrm{B}} \log \rho + \frac{1}{\theta_0} H = \alpha I$ implies the desired result. ∎

In general it seems difficult to exclude steady states $q = (\rho, \theta)$ with $\det \rho = 0$. We refer to Section 5.3 for an example where (4.14) does not hold and where a whole segment of equilibria exists for each E_0.

Open problem 2: *Provide minimal assumptions on* H, Q_m^n, *and* κ *to guarantee that there are no steady states with* $\det \rho = 0$.

4.4 Comparison to the Lindblad equation

Most often dissipative quantum mechanics is described in terms of the Lindblad equation (cf. [Lin76, Gra82, Lin83]). In the isothermal case $\theta_m = \theta_*$, (4.12a) takes the nonlinear form

$$\dot\rho = \jmath[\rho, H] - \sum_{m=1}^{M} \sum_{n=1}^{N_m} \big[Q_m^n, k_{\mathrm{B}}[Q_m^n, \rho] + \frac{1}{\theta_*} \mathcal{C}_\rho[Q_m^n, H]\big], \tag{4.15}$$

where now the free energy $\mathcal{F}_*(\rho) = k_{\mathrm{B}}\theta_* \langle\!\langle\, \rho \,\|\, \log \rho \,\rangle\!\rangle + \langle\!\langle\, \rho \,\|\, H \,\rangle\!\rangle$ is a Liapunov function.

The corresponding linear Lindblad equation is obtained from (4.15) simply by replacing $\mathcal{C}_\rho$ by $\mathcal{C}_{\rho_{\mathrm{eq}}}$ where we take the $\rho_\varepsilon = \frac{1}{Z} \exp\big(\frac{-1}{k_{\mathrm{B}}\theta_*} H\big)$. Using the commutator relation (4.5) we have $\mathcal{C}_{\rho_{\mathrm{eq}}}[Q_m^n, H] = -k_{\mathrm{B}}\theta[Q_m^n, \rho_{\mathrm{eq}}]$ and arrive at

$$\dot\rho = \jmath[\rho, H] - \sum_{m=1}^{M} \sum_{n=1}^{N_m} \big[\, Q_m^n \,,\, k_{\mathrm{B}}\,[Q_m^n \,,\, \rho - \rho_{\mathrm{eq}}\,]\,\big]. \tag{4.16}$$

The striking advantage of the Lindblad equation is its linearity. We will see in Section 6 that it also leaves $\mathfrak{R}$ invariant, i.e. it preserves the trace condition $\operatorname{tr}\rho = 1$, the symmetry $\rho = \rho^*$, and the positivity $\rho \geq 0$.

However, for the coupling to the exterior like heat baths it is less useful. Note that ρ_{eq} has to be known already. In general, the equilibrium ρ_{eq} will depend in a complicated and nonlinear way on the other variables, e.g. $\rho_{\mathrm{eq}}(\theta)$ in (4.12). More importantly, one has to model the influence of $\rho - \rho_{\mathrm{eq}}(\theta)$ on the other variables in a self-consistent way. In particular, energy conservation and nonnegative entropy production rates have to be guaranteed.

5 A simple coupled system

5.1 The case of one heat bath

We simplify the above problem even further, by assuming that there is only one dissipative interaction term (i.e. $m = 1$) with one coupling operator Q (i.e. $N_1 = 1$). Moreover, the matrix κ disappears as $c > 0$ and $\kappa c = 0$. The system reduces to

$$\begin{aligned} \dot\rho &= \jmath\big[H,\rho\big] - \Big[Q, k_{\mathrm{B}}\big[Q,\rho\big] + \frac{1}{\theta}\mathcal{C}_\rho\big[Q,H\big]\Big], \\ \dot\theta &= \frac{1}{c}\langle\!\langle\, k_{\mathrm{B}}\big[Q,\rho\big] + \frac{1}{\theta}\mathcal{C}_\rho\big[Q,H\big] \parallel \big[Q,H\big] \,\rangle\!\rangle. \end{aligned} \tag{5.1}$$

Energy and entropy are given by

$$\mathcal{E}(\rho,\theta) = \langle\!\langle\, \rho \parallel H \,\rangle\!\rangle + c\theta \quad \text{and} \quad \mathcal{S}(\rho,\theta) = -k_{\mathrm{B}}\operatorname{tr}(\rho\log\rho) + c\log\theta$$

It is easy to check that $\mathcal{E}$ is conserved along solutions while $\mathcal{S}$ is nondecreasing. For this, set $\Phi = -k_{\mathrm{B}}\log\rho - \frac{1}{\theta}H$, where Φ can be seen as the driving force for irreversible processes as $\mathrm{D}\mathcal{S} - \frac{1}{\theta}\mathrm{D}\mathcal{E} = (\Phi, 0)^{\mathsf{T}}$, see [Mie11a]. With these abbreviations system (5.1) takes the form

$$\dot\rho = \jmath\big[H,\rho\big] + \mathcal{K}_\rho^Q\Phi, \quad \dot\theta = -\frac{1}{c}\langle\!\langle\, \mathcal{K}_\rho^Q\Phi \parallel H \,\rangle\!\rangle.$$

Hence, we easily find

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(\rho(t),\theta(t)) &= \langle\!\langle\, \dot\rho \parallel H \,\rangle\!\rangle + c\dot\theta = 0 + \langle\!\langle\, \mathcal{K}_\rho^Q\Phi \parallel H \,\rangle\!\rangle - \langle\!\langle\, \mathcal{K}_\rho^Q\Phi \parallel H \,\rangle\!\rangle = 0, \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(\rho(t),\theta(t)) &= \langle\!\langle\, \dot\rho \parallel -k_{\mathrm{B}}\log\rho \,\rangle\!\rangle + c\frac{\dot\theta}{\theta} = 0 + \langle\!\langle\, \mathcal{K}_\rho^Q\Phi \parallel -k_{\mathrm{B}}\log\rho \,\rangle\!\rangle - \frac{1}{\theta}\langle\!\langle\, \mathcal{K}_\rho^Q\Phi \parallel H \,\rangle\!\rangle \\ &= \langle\!\langle\, \mathcal{K}_\rho^Q\Phi \parallel \Phi \,\rangle\!\rangle = \langle\!\langle\, \mathcal{C}_\rho\big[Q,\Phi\big] \parallel \big[Q,\Phi\big] \,\rangle\!\rangle \geq 0. \end{aligned}$$

5.2 Elimination of the temperature

Since $\theta > 0$ is only a scalar, we may eliminate it by using the invariance of the energy by assuming $\mathcal{E}(\rho,\theta) = E_0$. Then, $\theta = (E_0 - \langle\!\langle\, \rho \parallel H \,\rangle\!\rangle)/c$ and we can reduce system (5.1) to the single equation for ρ:

$$\dot\rho = \jmath\big[H,\rho\big] - \Big[Q, k_{\mathrm{B}}\big[Q,\rho\big] + \frac{c}{E_0 - \langle\!\langle\, \rho \parallel H \,\rangle\!\rangle}\,\mathcal{C}_\rho\big[Q,H\big]\Big], \tag{5.2a}$$

which has the negative entropy $-\widetilde{\mathcal{S}}$ as a Liapunov functional, where

$$\widetilde{\mathcal{S}}(\rho) = -k_{\mathrm{B}}\langle\!\langle\, \rho \,\|\, \log\rho \,\rangle\!\rangle + c\log\big(E_0 - \langle\!\langle\, \rho \,\|\, H \,\rangle\!\rangle\big). \tag{5.2b}$$

Note that $\widetilde{\mathcal{S}}$ is still a strictly concave function on the compact set $\mathfrak{R}$. Hence, assuming that E_0 is given such that $\widetilde{\mathcal{S}}$ is finite at least at one point in $\mathfrak{R}$, then there is a unique maximizer ρ_* given via

$$\theta_* = (E_0 - \langle\!\langle\, \rho_* \,\|\, H \,\rangle\!\rangle)/c > 0 \quad \text{and} \quad \rho_* = \frac{1}{Z}\exp\big(-\tfrac{1}{k_{\mathrm{B}}\theta_*}H\big). \tag{5.3}$$

In fact, we are now easily able to pass to the isothermal limit in the sense of Section 2.3. We assume that E_0 and c tend to ∞ while H and Q are fixed. Assuming $E_0/c \to \theta_* > 0$ we find the expansion

$$c\log\big(E_0 - \langle\!\langle\, \rho \,\|\, H \,\rangle\!\rangle\big) = c\log E_0 - \frac{c}{E_0}\langle\!\langle\, \rho \,\|\, H \,\rangle\!\rangle + O(c/E_0^2),$$

where we use that $\rho \in \mathfrak{R}$ is bounded. Thus, we find the free energy

$$\mathcal{F}_*(\rho) = \lim_{\substack{c,E_0\to\infty \\ E_0/c\to\theta_*}} \Big(E_0\log E_0 - \theta_*\widetilde{\mathcal{S}}(\rho)\Big) = \langle\!\langle\, \rho \,\|\, H \,\rangle\!\rangle + k_{\mathrm{B}}\theta_*\langle\!\langle\, \rho \,\|\, \log\rho \,\rangle\!\rangle, \tag{5.4a}$$

and the simplified isothermal evolutionary system

$$\dot\rho = \jmath\big[H,\rho\big] - \Big[Q, k_{\mathrm{B}}\big[Q,\rho\big] + \frac{1}{\theta_*}\mathcal{C}_\rho\big[Q,H\big]\Big]. \tag{5.4b}$$

5.3 The case $\dim \boldsymbol{H} = 2$

In the case that the basic Hilbert space $\boldsymbol{H}$ is two-dimensional, i.e. $\boldsymbol{H} = \mathbb{C}^2$, we can write (5.4) explicitly by introducing suitable coordinates. While in the general case $\boldsymbol{H} = \mathrm{C}^n$ the set $\mathfrak{R}$ can be seen as a real (n^2-1)-dimensional manifold with piecewise smooth boundary, the case $n = 2$ is special, because $\mathfrak{R}$ has a smooth boundary and can be identified by the closed ball $\mathcal{A} = B_{1/2}(0) \subset \mathbb{R}^3$ as follows:

$$\mathfrak{R} = \{\, \rho = \widehat\rho(\boldsymbol{a}) \mid \boldsymbol{a} \in \mathcal{A}\,\}, \quad \text{where } \widehat\rho(\alpha,\beta,\gamma) = \begin{pmatrix} \frac{1}{2}+\alpha & \beta+\mathrm{i}\gamma \\ \beta-\mathrm{i}\gamma & \frac{1}{2}-\alpha \end{pmatrix}.$$

Using $z = \beta + \jmath\gamma$ and $r = |\boldsymbol{a}|$ the eigenvalues $r_\pm$ and eigenvectors $\psi_\pm$ of $\widehat\rho(\boldsymbol{a})$ are

$$r_\pm = \frac{1}{2} \pm r, \qquad \psi_\pm = \frac{1}{\sqrt{2r(r\mp\alpha)}}\begin{pmatrix} z \\ -\alpha \pm r \end{pmatrix}.$$

Thus, $\mathcal{C}_{\widehat\rho(\boldsymbol{a})}$ can be written out explicitly using (4.2). In particular, choosing H and Q we are able to write (5.2) and (5.4b) as explicit ODE systems in the three variables (α,β,γ). For didactical purposes we will do this for the special case

$$H = \begin{pmatrix} h_1 & 0 \\ 0 & h_2 \end{pmatrix} \quad \text{and} \quad Q = \begin{pmatrix} 0 & q \\ q & 0 \end{pmatrix},$$

where $h_1, h_2, q \in R$. In treating this example, we will see some of the difficulties in proofing the existence of solutions and the convergence of all solutions into the unique thermodynamic equilibrium ρ_*. We first note that the free energy $\mathcal{F}_*$ has the form

$$\widehat{\mathcal{F}}(\boldsymbol{a}) = \mathcal{F}_*(\widehat{\rho}(\boldsymbol{a})) = k_{\mathrm{B}}\theta_*\big((\tfrac{1}{2}{+}r)\log(\tfrac{1}{2}{+}r) + (\tfrac{1}{2}{-}r)\log(\tfrac{1}{2}{-}r)\big) + \tfrac{1}{2}(h_1{+}h_2) - (h_2{-}h_1)\alpha.$$

Some lengthy calculations, using the explicit form of $r_\pm$, $\psi_\pm$ and (4.2), give

$$\mathcal{C}_{\widehat{\rho}(\boldsymbol{a})}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} -\mathrm{i}\gamma\big(1 + \frac{1-2\lambda}{2r^2}\alpha\big) & \lambda{+}\frac{1-2\lambda}{2r^2}\gamma^2 - \mathrm{i}\frac{1-2\lambda}{2r^2}\beta \\ -\lambda{-}\frac{1-2\lambda}{2r^2}\gamma^2 - \mathrm{i}\frac{1-2\lambda}{2r^2}\beta & \mathrm{i}\gamma\big(\frac{1-2\lambda}{2r^2}\alpha - 1\big) \end{pmatrix},$$

where $\lambda = \lambda(r) = \Lambda(\frac{1}{2}{+}r, \frac{1}{2}{-}r)$. Using $\lambda(0) = 1/2$ we see that $r \mapsto (\lambda(r), \frac{1-2\lambda(r)}{2r^2})$ is analytic on $[0, 1/2[$ and continuous on $[0, 1/2]$. Thus, we see that $\boldsymbol{a} \mapsto \mathcal{C}_{\widehat{\rho}(\boldsymbol{a})}\left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$ is smooth in the interior of $\mathcal{A}$ and continuous on the closed ball $\mathcal{A}$, as predicted by Proposition 4.2. Inserting this into (5.4b) leads to the system

$$\begin{pmatrix} \dot\alpha \\ \dot\beta \\ \dot\gamma \end{pmatrix} = \begin{pmatrix} 0 \\ (h_2{-}h_1)\gamma \\ (h_1{-}h_2)\beta \end{pmatrix} - k_{\mathrm{B}}q^2 \begin{pmatrix} 4\alpha \\ 0 \\ 4\gamma \end{pmatrix} + \frac{q^2(h_2{-}h_1)}{\theta_*} \begin{pmatrix} 2\lambda{+}\frac{1-2\lambda}{r^2}\gamma^2 \\ 0 \\ -\frac{1-2\lambda}{r^2}\alpha\gamma \end{pmatrix}. \tag{5.5}$$

It is also instructive to see the isothermal form of the GENERIC system as given in (2.10). Using the coordinates $\boldsymbol{a} = (\alpha, \beta, \gamma)^{\mathsf{T}} \in \mathcal{A}$ and $r = |\boldsymbol{a}|$ we have

$$\mathrm{D}\widehat{\mathcal{F}}(a) = \frac{2k_{\mathrm{B}}\theta_*}{\lambda(r)} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} - \begin{pmatrix} h_2{-}h_1 \\ 0 \\ 0 \end{pmatrix}, \quad \widehat{J}(\boldsymbol{a}) = \begin{pmatrix} 0 & \gamma & -\beta \\ -\gamma & 0 & \alpha \\ \beta & -\alpha & 0 \end{pmatrix},$$
$$\widehat{K}(\boldsymbol{a}) = q^2 \begin{pmatrix} 2\lambda(r) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2\lambda(r) \end{pmatrix} + \frac{q^2(1{-}2\lambda(r))}{r^2} \begin{pmatrix} \gamma^2 & 0 & -\alpha\gamma \\ 0 & 0 & 0 \\ -\alpha\gamma & 0 & \alpha^2 \end{pmatrix}.$$

It is now easy to see that (5.5) is given in the form $\dot{\boldsymbol{a}} = \big(\widehat{J}(\boldsymbol{a}) - \frac{1}{\theta_*}\widehat{K}(\boldsymbol{a})\big)\mathrm{D}\widehat{\mathcal{F}}(\boldsymbol{a})$. Moreover, we see that the Poisson structure $\widehat{J}$ on $\mathcal{A}$ is the classical Lie-Poisson structure on $\mathbb{R}^3$ used for Euler's equation for rigid bodies, cf. [AbM78, MaR99]. Moreover, we see that there is no dissipation in the β-component, since its direction is parallel to Q and, thus, vanishes in the commutator.

In particular, we see that all solutions starting in $\mathcal{A}$ remain there. In fact,

$$\tfrac{1}{2}\tfrac{\mathrm{d}}{\mathrm{d}t}r^2 = \tfrac{1}{2}\tfrac{\mathrm{d}}{\mathrm{d}t}|\boldsymbol{a}|^2 = \boldsymbol{a}\cdot\dot{\boldsymbol{a}} = -4k_{\mathrm{B}}q^2(\alpha^2{+}\gamma^2) + \tfrac{2q^2}{\theta_*}(h_2{-}h_1)\alpha\lambda(|\boldsymbol{a}|) \tag{5.6}$$

implies that for $\boldsymbol{a} \in \partial\mathcal{A}$ (i.e. $r = |\boldsymbol{a}| = 1/2$) we have $\dot r \le 0$ because of $\lambda(1/2) = 0$. Moreover, solutions immediately move into the interior of $\mathcal{A}$ except when starting in $\boldsymbol{a}(0) = (0, \pm 1/2, 0)^{\mathsf{T}}$, where $\dot{\boldsymbol{a}} = \pm(0, 0, (h_1{-}h_2)/2)^{\mathsf{T}}$. Hence, except for the case $h_1 = h_2$ also in this case the solutions leave the boundary of $\mathcal{A}$.

The following general result on the dynamics of the simple ODE system (5.5) is an immediate consequence of the above derivations.

Theorem 5.1 *System* (5.5) *has for each initial condition $\boldsymbol{a}(0) \in \mathcal{A}$ a global solution, along which $\widehat{\mathcal{F}}$ is nonincreasing. Solutions with $|\boldsymbol{a}(0)| < 1/2$ are unique and never touch the boundary $\partial\mathcal{A}$.*

In the purely Hamiltonian case $q = 0$ the solution are periodic with $\alpha(t) = \alpha(0)$ and $r(t) = r(0)$, i.e. the free energy $\widehat{\mathcal{F}}(\boldsymbol{a}(t))$ is constant.

For $q \neq 0$ all solutions $\boldsymbol{a}(t)$ converge to a steady state for $t \to \infty$. If $h_1 \neq h_2$ this is the unique steady state $\boldsymbol{a}_*$ corresponding to $\rho_* = \widehat{\rho}(\boldsymbol{a}_*)$ given in (5.3) *and minimizing $\widehat{\mathcal{F}}$.*

If $h_1 = h_2$, then $\beta(t) = \beta(0)$ while $(\alpha(t), \gamma(t)) = \mathrm{e}^{-4k_{\mathrm{B}}q^2 t}(\alpha(0), \gamma(0))$.

Finally, we compare the solutions of the GENERIC system (5.5) with the corresponding linear Lindblad system, where the nonlinear term $[Q, \mathcal{C}_\rho[Q, H]]$ is replaced by the constant term $[Q, \mathcal{C}_{\rho_{\mathbf{eq}}}[Q, H]] = -k_{\mathrm{B}}\theta_*[Q, [Q, \rho_{\mathbf{eq}}]] =$ const. in (5.4b), namely

$$\begin{pmatrix} \dot\alpha \\ \dot\beta \\ \dot\gamma \end{pmatrix} = \begin{pmatrix} 0 \\ (h_2{-}h_1)\gamma \\ (h_1{-}h_2)\beta \end{pmatrix} - 4k_{\mathrm{B}}q^2 \begin{pmatrix} \alpha - \alpha_{\mathbf{eq}} \\ 0 \\ \gamma \end{pmatrix}, \tag{5.7}$$

where $\alpha_{\mathbf{eq}}$ depends on θ_* and $h_2{-}h_1$. Note that the dynamics of α and (β, γ) are mutually uncoupled, which is certainly not the case in (5.5).

6 Existence and convergence into equilibrium

Here we restrict ourselves to the finite-dimensional setting assuming $\boldsymbol{H} = \mathbb{C}^n$ for $n \geq 2$. To keep notations simple we study the case without temperature, i.e. we either consider the isothermal case (5.4) or the full case (5.2) for a given value of E_0, see Section 5.2. In both cases the driving functional (now being a Liapunov functional) has the form

$$\mathcal{F}(\rho) = e\,\langle\!\langle\, \rho \,\|\, \log\rho \,\rangle\!\rangle + m(\langle\!\langle\, \rho \,\|\, H \,\rangle\!\rangle),$$

where $e > 0$ and $m : \mathbb{R} \to \mathbb{R} \cup \{\infty\}$ is continuous convex function. Our state space is the compact set $\mathfrak{R}$ and the equation we study is

$$\begin{aligned} \dot\rho = \mathcal{V}(\rho) &:= \jmath[H, \rho] - \sum_{n=1}^{N} \big[Q^n, \mathcal{C}_\rho[Q^n, \mathrm{D}\mathcal{F}(\rho)]\big] \\ &= \jmath[H, \rho] - e\sum_{n=1}^{N} \big[Q^n, [Q^n, \rho]\big] - m'(\langle\!\langle\, \rho \,\|\, H \,\rangle\!\rangle) \sum_{n=1}^{N} \big[Q^n, \mathcal{C}_\rho[Q^n, H]\big]. \end{aligned} \tag{6.1}$$

6.1 Existence via a modified explicit Euler scheme

The construction of solutions uses an explicit Euler scheme with a slight modification to keep the property $\rho \in \mathfrak{R}$. Consider the time interval $[0, t_0]$, choose an integer N, and define the time step $\delta = t_0/N$. For a given initial condition q_0 we define incrementally

$$\rho^{k+1} = \mathcal{P}_{\mathfrak{R}}\big(\rho^k + \delta\mathcal{V}(\rho^k)\big). \tag{6.2}$$

Here we introduced the projection operator $\mathcal{P}_{\mathfrak{R}}$ that maps arbitrary matrices with trace 1 to elements in $\mathfrak{R}$ in the following way

$$\mathcal{P}_{\mathfrak{R}}\Big(\sum_{i=1}^{n} r_j\psi_i\otimes\overline{\psi}_i\Big) = \tfrac{1}{\sum_{i=1}^{n}\max\{0,r_j\}}\sum_{i=1}^{n}\max\{0,r_j\}\psi_i\otimes\overline{\psi}_i.$$

The necessary properties of $\mathcal{P}_{\mathfrak{R}}$ are given in the following lemma.

Lemma 6.1 *The nonlinear projector $\mathcal{P}_{\mathfrak{R}}$ satisfies:*

(i) $\exists\, C>0\ \forall\, \rho_1,\rho_2\in\mathbb{C}_{\mathrm{S}}^{n\times n}$ *with* $\operatorname{tr}\rho_j=1$*:*
$\operatorname{dist}(\rho_j,\mathfrak{R})\le 1/2 \implies \|\mathcal{P}_{\mathfrak{R}}(\rho_1)-\mathcal{P}_{\mathfrak{R}}(\rho_2)\|\le C\|\rho_1-\rho_2\|.$

(ii) If $\mathfrak{R}\ni\rho^k\to\rho\in\mathfrak{R}$*, and* $\delta^k\to 0$*, then* $\frac{1}{\delta_k}\big(\mathcal{P}_{\mathfrak{R}}\big(\rho^k+\delta_k\mathcal{V}(\rho^k)\big)-\rho^k\big)\ \to\ \mathcal{V}(\rho)$.

Proof: Assertion (i) is clear by the classical Lipschitz continuity of orthogonal projections.

For assertion (ii) we distinguish the cases $\rho>0$ and $\rho\in\partial\mathfrak{R}$. In the first case convergence (ii) follows easily by the continuity of $\mathcal{V}$, because for sufficiently large k the projection $\mathcal{P}_{\mathfrak{R}}$ acts as identity.

Now assume $\rho=\left(\begin{smallmatrix}\sigma & 0\\ 0 & 0\end{smallmatrix}\right)$ with $\sigma>0$. In particular, we split the space $\boldsymbol{H}=\boldsymbol{H}_1\oplus\boldsymbol{H}_2$ and write all operators as 2×2-block operators with respect to this splitting. We find

$$\mathcal{C}_\rho\begin{pmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{pmatrix}=\begin{pmatrix}\mathcal{C}_\sigma A_{11} & 0\\ 0 & 0\end{pmatrix} \tag{6.3}$$

and conclude that $\mathcal{V}(\rho)=\left(\begin{smallmatrix}\alpha & \beta\\ \beta^* & 0\end{smallmatrix}\right)$. To show (ii) we use the decomposition

$$\begin{aligned}
&\tfrac{1}{\delta_k}\Big(\mathcal{P}_{\mathfrak{R}}\big(\rho^k+\delta_k\mathcal{V}(\rho^k)\big)-\rho^k\Big)=V_k^1+V_k^2+\mathcal{V}(\rho),\\
&\text{where } V_k^1:=\tfrac{1}{\delta_k}\Big(\mathcal{P}_{\mathfrak{R}}\big(\rho^k+\delta_k\mathcal{V}(\rho^k)\big)-\mathcal{P}_{\mathfrak{R}}\big(\rho^k+\delta_k\mathcal{V}(\rho)\big)\Big)\\
&\text{and}\quad V_k^2:=\tfrac{1}{\delta_k}\Big(\mathcal{P}_{\mathfrak{R}}\big(\rho^k+\delta_k\mathcal{V}(\rho)\big)-\big(\rho^k+\delta_k\mathcal{V}(\rho)\big)\Big),
\end{aligned}$$

which means that we have to show $V_k^1\to 0$ and $V_k^2\to 0$. By the Lipschitz continuity (i) and the continuity of $\mathcal{V}$ on $\mathfrak{R}$ we have $\|V_k^1\|\le C\|\mathcal{V}(\rho^k)-\mathcal{V}(\rho)\|\to 0$.

For the second term we establish the decomposition

$$\rho_k:=\rho^k+\delta_k\mathcal{V}(\rho)=\widetilde{\rho}_k+\delta_k W_k\quad\text{with }\widetilde{\rho}_k\in\mathfrak{R}\text{ and }W_k\to 0. \tag{6.4}$$

Then, $\mathcal{P}_{\mathfrak{R}}(\widetilde{\rho}_k)=\widetilde{\rho}_k$ implies the estimate

$$\|V_k^2\|=\tfrac{1}{\delta_k}\|\mathcal{P}_{\mathfrak{R}}(\rho_k)-\rho_k\|\le\tfrac{1}{\delta_k}\|\mathcal{P}_{\mathfrak{R}}(\rho_k)-\mathcal{P}_{\mathfrak{R}}(\widetilde{\rho}_k)\|+\tfrac{1}{\delta_k}\|\widetilde{\rho}_k-\rho_k\|\le(C+1)\|W_k\|\to 0,$$

which establishes the convergence in (ii).

It remains to show (6.4). We use the notation

$$\rho^k=\begin{pmatrix}\sigma_k & b_k\\ b_k^* & c_k\end{pmatrix}\text{ and }\rho_k=\rho^k+\delta_k\mathcal{V}(\rho)=\begin{pmatrix}\Sigma_k & B_k\\ B_k^* & c_k\end{pmatrix},$$

i.e. $\Sigma_k = \sigma_k + \delta_k\alpha$ and $B_k = b_k + \delta_k\beta$. As an intermediate decomposition we let

$$\rho_k = \widehat{\rho}_k + \begin{pmatrix} 0 & 0 \\ 0 & \delta_k\gamma_k \end{pmatrix}, \text{ where } \gamma_k = \tfrac{1}{\delta_k}\big(b_k^*\sigma_k^{-1}b_k - B_k^*\Sigma_k^{-1}B_k\big).$$

Here $\widehat{\rho}_k$ is positive semidefinite because of

$$\widehat{\rho}_k = \begin{pmatrix} \Sigma_k & B_k \\ B_k^* & B_k^*\Sigma_k^{-1}B_k \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & c_k - b_k^*\sigma_k^{-1}b_k \end{pmatrix},$$

where the first and second operator are positive semidefinite because of $\sigma \approx \Sigma_k > 0$ and $\rho^k \geq 0$, respectively. Using $\operatorname{tr}\widehat{\rho}_k = 1 - \delta_k \operatorname{tr}\gamma_k \approx 1$, we now let

$$\rho_k = \widetilde{\rho}_k + \delta_k W_k \quad \text{with } \widetilde{\rho}_k = \tfrac{1}{1-\delta_k \operatorname{tr}\gamma_k}\,\widehat{\rho}_k \text{ and } W_k = \begin{pmatrix} 0 & 0 \\ 0 & \gamma_k \end{pmatrix} - (\operatorname{tr}\gamma_k)\,\widetilde{\rho}_k.$$

By construction we have $\rho \approx \widetilde{\rho}_k \in \mathfrak{R}$ and it remains to be shown $\gamma_k \to 0$. Using $\rho^k \to 0$ we have $b_k \to 0$ and, hence, obtain

$$\|\gamma_k\| \leq \frac{C_1}{\delta_k}\big(\|B_k - b_k\|(\|b_k\| + \|B_k\|) + \|\sigma_k - \Sigma_k\|(\|B_k\| + \|b_k\|)^2\big) \leq C_2(\|b_k\| + \delta_k) \to 0.$$

This completes the proof of the lemma. ∎

With this lemma at hand, we obtain our global existence result. In contrast to the subsequent convergence result, we don't need any specific properties of H, Q^1, ..Q^N. In [MiN12] we will show that the existence result can be extended to more general systems containing several heat baths, e.g. (4.12).

Theorem 6.2 *Consider e, m, H, and arbitrary coupling operators Q^n as defined at the beginning of this section. Then, for all initial conditions $\rho^0 \in \mathfrak{R}$ there is a global solution $\rho \in \mathrm{C}^1([0,\infty[\,;\mathfrak{R})$ of* (6.1) *with $\rho(0) = \rho^0$.*

Proof: The proof follows easily using the incremental approach based on the modified explicit Euler scheme (6.2). Since the vector field $\mathcal{V}$ is continuous on the compact set $\mathfrak{R}$ it is bounded. For a given time increment $\delta > 0$ we obtain the incremental approximations ρ_δ^k and form two interpolants, namely $\widehat{\rho}_\delta : [0,\infty[\to \mathfrak{R}$ and $\overline{\rho}_\delta : [0,\infty[\to \mathfrak{R}$, where $\widehat{\rho}_\delta$ is continuous and piecewise affine, whereas $\overline{\rho}_\delta$ is piecewise constant and continuous from the right, i.e. $\overline{\rho}_\delta(t) = \rho_\delta^k$ for $k\delta \leq t < (k+1)\delta$. Obviously, these interpolants satisfy

$$\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\rho}_\delta(t) = \tfrac{1}{\delta}\Big(\mathcal{P}_{\mathfrak{R}}\big(\overline{q}_\delta + \delta\mathcal{V}_{\mathfrak{R}}(\overline{q}_\delta)\big) - \overline{q}_\delta\Big) \quad \text{for all } t \in [0,\infty[\,\setminus\,\{\,\delta k \mid k \in \mathbb{N}\,\}. \tag{6.5}$$

Moreover, the sequence $\widehat{\rho}_\delta$ is uniformly Lipschitz continuous and, thus, admits a uniformly converging subsequence with $\delta = \delta_k \to 0$ and a limit $q : [0,t_0] \to \mathcal{Q}$. Moreover, we may assume $\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\rho}_\delta \overset{*}{\rightharpoonup} w$ in $\mathrm{L}^\infty([0,\infty[;\mathrm{L}^2_{\mathrm{S}}(\boldsymbol{H}))$. Using Lemma 6.1 and the uniform convergence of ρ_δ to ρ, the right-hand side in (6.5) converges uniformly to $\mathcal{V}(\rho(t))$. Standard ODE arguments show that $\rho \in \mathrm{C}^1([0,\infty[;\mathrm{L}^2_{\mathrm{S}}(\boldsymbol{H}))$ with $\dot{\rho} = w$, such that $\dot{\rho} = \mathcal{V}(\rho)$. Hence, ρ is a solution of (6.1). ∎

Open problem 3: *Do we have uniqueness if every solution leave, the boundary of $\mathfrak{R}$ immediately? What are conditions on H and Q^n to guarantee this property?*

6.2 Convergence into the thermodynamic equilibrium

One problem in our system is that the functional $\mathcal{F}$ (or more general the entropy $\mathcal{S}(\rho,\theta)$) is not differentiable on the boundary $\partial\mathfrak{R}$ of $\mathfrak{R}$. Thus, it is not clear how to show that $\mathcal{F}$ is a strict Liapunov function along solutions staying on $\partial\mathfrak{R}$. Thus, we will first provide some general conditions on the coupling operators Q^n such that $\partial\mathfrak{R}$ is transversally repelling, i.e. each solution leaves the boundary to the inside with a positive speed.

For a family $\boldsymbol{Q} = (Q^1, ..., Q^N) \in \mathrm{L}^2_{\mathrm{S}}(\boldsymbol{H})^N$ we define

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

Clearly, we have $\mu(\boldsymbol{Q})$ if $\boldsymbol{Q} = (Q)$ and $\dim \boldsymbol{H} \geq 2$, since then we may choose two orthogonal eigenvectors of Q. However, for $\boldsymbol{Q} = (Q^1, Q^2)$ with

$$Q^1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{ and } Q^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

we find $\mu(\boldsymbol{Q}) > 0$.

Open problem 4: *What is the minimal number N for a given $\dim \boldsymbol{H}$ such that there exists $\boldsymbol{Q} = (Q^1, ..., Q^N)$ with $\mu(\boldsymbol{Q}) > 0$?*

Proposition 6.3 *Assume that* (6.1) *satisfies additionally $\mu(\boldsymbol{Q}) > 0$, then all solutions $\rho : [0,\infty[\to \mathfrak{R}$ with $\rho(0) \in \operatorname{int}\mathfrak{R}$ satisfy $\inf\{\, \operatorname{dist}(\rho(t), \partial\mathfrak{R}) \mid t \geq 0 \,\} > 0$. Moreover, there exist $t_0 > 0$ such that for each solutions with $\rho(0) \in \partial\mathfrak{R}$ we have $\operatorname{dist}(\rho(t), \partial\mathfrak{R}) \geq e\mu(\boldsymbol{Q})t > 0$ for $t \in]0, t_0]$.*

Proof: Since $\rho = \sum_{k=1}^{\dim \boldsymbol{H}} r_k \psi_k \otimes \overline{\psi}_k$ we have $\rho \in \partial\mathfrak{R}$ if and only if $\det \rho = \prod_{k=1}^{\dim \boldsymbol{H}} r_k = 0$. This implies $\operatorname{dist}(\rho, \partial\mathfrak{R}) \geq \min\{\, r_k \mid k = 1, .., \dim \boldsymbol{H} \,\}$. Moreover, from the equation $\dot\rho = \mathcal{V}(\rho)$ and $\rho(t) = \sum_{k=1}^{\dim \boldsymbol{H}} r_k(t)\psi_k(t) \otimes \overline{\psi}_k(t)$ we obtain easily the relation

$$\dot r_k(t) = \langle\!\langle\, \mathcal{V}(\rho(t)) \,\|\, \psi_k(t) \otimes \overline{\psi}_k(t) \,\rangle\!\rangle = \langle \mathcal{V}(\rho(t))\psi_k(t) | \psi_k(t)\rangle.$$

Now assume $\rho(t) \in \partial\mathfrak{R}$, which means that there exists k with $r_k(t) = 0$. For the three terms of $\mathcal{V}$ in (6.1) we obtain $\langle\!\langle\, [\rho, H] \,\|\, \psi_k(t) \otimes \overline{\psi}_k(t) \,\rangle\!\rangle = \langle\!\langle\, H \,\|\, [\rho, \psi_k(t) \otimes \overline{\psi}_k(t)] \,\rangle\!\rangle = 0$ using (3.3). Invoking the block structure (6.3) with $\boldsymbol{H}_2 = \operatorname{span}\psi_k$ we find $(\mathcal{C}_\rho A)\psi_k(t) \otimes \overline{\psi}_k(t) = \psi_k(t) \otimes \overline{\psi}_k(t)(\mathcal{C}_\rho A) = 0$ for all A and conclude

$$\langle\!\langle\, [Q, \mathcal{C}_\rho B] \,\|\, \psi_k(t) \otimes \overline{\psi}_k(t) \,\rangle\!\rangle = \langle\!\langle\, [\mathcal{C}_\rho B, \psi_k(t) \otimes \overline{\psi}_k(t)] \,\|\, Q \,\rangle\!\rangle = \langle\!\langle\, 0 - 0 \,\|\, Q \,\rangle\!\rangle = 0.$$

Thus, only the Lindblad terms in $\mathcal{V}(\rho)$ remain. Using the abbreviation $E_j = \psi_j(t) \otimes \overline{\psi}_j(t)$ and $r_k(t) = 0$ we obtain the relation

$$\dot r_k(t) = -e\sum_{n=1}^{N} \langle\!\langle\, [Q^n, [Q^n, \rho]] \,\|\, E_k \,\rangle\!\rangle = -e \sum_{j=1}^{\dim \boldsymbol{H}} r_k \sum_{n=1}^{N} \langle\!\langle\, [Q^n, [Q^n, E_k]] \,\|\, E_k \,\rangle\!\rangle$$

$$= 2e \sum_{j\neq k} r_k \sum_{n=1}^{N} |\langle Q^n\psi_j|\psi_k\rangle|^2 \geq 2e \sum_{j\neq k} r_k\, \mu(\boldsymbol{Q}) = 2e\mu(\boldsymbol{Q}),$$

where we used $r_k = 0$ to drop the term for $j = k$ and $\langle\!\langle\, [Q,[Q,E_j]] \,\|\, E_k \,\rangle\!\rangle = -2|\langle Q\Psi_j|\Psi_k\rangle|^2$ for $j \neq k$. By the assumptions $e > 0$ and $\mu(\boldsymbol{Q}) > 0$ and the compactness of $\partial\mathfrak{R}$, the continuity of $\mathcal{V}$ guarantees that $\dot{r}_k(t) \geq e\mu(\boldsymbol{Q}) > 0$ whenever $\operatorname{dist}(\rho(t), \partial\mathfrak{R}) \leq \delta$ for some $\delta > 0$. Now all the assertions of the proposition follow by standard ODE arguments. ∎

The above proposition shows that we only need to consider solutions lying in the interior of $\mathfrak{R}$, where $\mathcal{F}$ is smooth and where the dissipation relation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(\rho(t)) = -2\Psi^*(\rho, \mathrm{D}\mathcal{F}(\rho)) = -\sum_{n=1}^{N} \|\!| \big[Q^n, e\log\rho + m'(\langle\!\langle\, \rho \,\|\, H \,\rangle\!\rangle)H\big] |\!\|_{\mathcal{C}_\rho}^2$$

holds. Hence, $\mathcal{F}$ is a Liapunov function but not necessarily a strict Liapunov function. The latter means that $\mathcal{F}$ is strictly decreasing along $t \mapsto \rho(t)$ whenever ρ is not constant (recall that we have uniqueness of solutions in the interior of $\mathfrak{R}$). In fact, (6.1) still allows for (linear) Hamiltonian dynamics in a subspace $\boldsymbol{H}_0$ if this subspace is left invariant by H and $Q^n|_{\boldsymbol{H}_0} = 0$ for all n.

The following result shows that a slight strengthening of the commutator condition (4.14), which was used to establish the uniqueness of steady states, is sufficient to show that $\mathcal{F}$ is a strict Liapunov function.

Theorem 6.4 *Assume that the system* (6.1) *satisfies* $\mu(\boldsymbol{Q}) > 0$ *and the strengthened commutator relation*

$$A \in \mathrm{L}^2_{\mathrm{S}}(\boldsymbol{H}) \text{ and } \forall\, n = 1, ..., N\colon [Q^n, A] = 0 \quad \Longrightarrow \quad \exists\, \alpha \in \mathbb{R}\colon A = \alpha I. \tag{6.6}$$

Then, all solutions $\rho : [0,\infty[\to \mathfrak{R}$ *of* (6.1) *satisfy* $\rho(t) \to \rho_{\mathrm{eq}}$*, where* ρ_{eq} *is the unique minimizer of* $\mathcal{F}$*.*

Proof: It remains to show that $\mathcal{F}$ is a strict Liapunov function. For this we have to investigate the set $\Psi^*(\rho, \mathrm{D}\mathcal{F}(\rho)) = 0$. Using $\mathcal{C}_\rho > 0$ for $\rho \in \operatorname{int}\mathcal{R}$ condition (6.6) gives $e\log\rho + m'(..)H = \alpha I$. Thus, we have $\rho = c\exp(-\gamma H)$ with $e\gamma = m'(\langle\!\langle\, \rho \,\|\, H \,\rangle\!\rangle)$, where $c > 0$ and $\gamma \in \mathbb{R}$ have to satisfy $1 = c\operatorname{tr}\exp(-\gamma H)$ and $e\gamma = m'(c\langle\!\langle \exp(-\gamma H) \,\|\, H \,\rangle\!\rangle)$. Because of the monotonicity of m' (convexity of m) there is exactly one solution which defines ρ_{eq}. Now, the convergence to the unique steady state follows by the principle of Krasovskii and La Salle, cf. [HiS74]. ∎

Open problem 5: *What are weaker conditions that guarantee that all solutions converge into some steady state? When is* $\mathcal{F}$ *a strict Liapunov function?*

7 Comparison to stochastic gradient structures

In this section we restrict ourselves to purely dissipative systems, which don't have any Hamiltonian part $J\mathrm{D}E$. Our aim is to highlight analogies between the dissipative evolution of the density operator ρ and certain other gradient flows arising in probabilistic systems. First, we compare to the Fokker-Planck equation with the Wasserstein gradient structure introduced in [JKO98, Ott01]. Second, we show the analogy to the entropic gradient structure for reversible Markov chains introduced in [Maa11, Mie11b].

In general, a gradient system consists of a basic space $\boldsymbol{X}$ with a differential structure, a differential potential $\mathcal{F} : \boldsymbol{X} \to \mathbb{R}$, and a metric $\mathcal{G}$ such that $\mathcal{G}(u) : \mathrm{T}_u\boldsymbol{X} \to \mathrm{T}_u^*\boldsymbol{X}$ is a linear, symmetric, and positive definite operator. As in the GENERIC framework we will use the the inverse operator $\mathcal{K}(u) = \mathcal{G}(u)^{-1}$ and will denote the gradient system by $(\boldsymbol{X}, \mathcal{F}, \mathcal{K})$. The gradient flow is then defined by the evolutionary equation

$$0 = \mathcal{G}(u)\dot{u} + \mathrm{D}\mathcal{F}(u) \quad \Longleftrightarrow \quad \dot{u} = -\nabla_{\mathcal{G}}\mathcal{F}(u) =: -\mathcal{K}(u)\mathrm{D}\mathcal{F}(u).$$

Thus neglecting the Hamiltonian part $\jmath[\rho, H]$ in our dissipative quantum system (6.1) we have the gradient system $(\mathfrak{R}, \mathcal{F}_{\mathrm{qm}}, \mathcal{K}_{\mathrm{qm}}^{\boldsymbol{Q}})$ with

$$\mathcal{F}_{\mathrm{qm}}(\rho) := \langle\!\langle\, \rho \,\|\, \log \rho \,\rangle\!\rangle + \langle\!\langle\, \rho \,\|\, H \,\rangle\!\rangle \quad \text{and } \mathcal{K}_{\mathrm{qm}}^{\boldsymbol{Q}}(\rho)\Xi := \sum_{n=1}^{N} \big[Q^n, \mathcal{C}_\rho[Q^n, \Xi]\big].$$

Hence, $\mathcal{K}_{\mathrm{qm}}^{\boldsymbol{Q}}$ is associated with the dual dissipation potential $\Psi_{\mathrm{qm}}^*(\rho, \Xi) = \frac{1}{2}\sum_1^N \|[Q^n, \Xi]\|_{\mathcal{C}_\rho}^2$.

We now compare this with the Fokker-Planck equation

$$\dot{u} = \operatorname{div}(M(\nabla u + u\nabla H)), \quad t > 0,\ x \in \mathbb{R}^d,$$

where $M \in \mathbb{R}^{d\times d}$ is a symmetric and positive definite matrix and $H \in \mathrm{C}^2(\mathbb{R}^d)$ is a suitable potential. This equation can be understood as the gradient system $(\mathrm{L}^2(\mathbb{R}^d), \mathcal{F}_{\mathrm{FP}}, \mathcal{K}_{\mathrm{FP}})$ with

$$\mathcal{F}_{\mathrm{FP}}(u) := \int_{\mathbb{R}^d} u\log u + uH \,\mathrm{d}x \quad \text{and} \quad \mathcal{K}_{\mathrm{FP}}(u)\xi := -\sum_{i,j} \partial_{x_i}\big(uM_{ij}\partial_{x_j}\xi\big).$$

The analogy between $\mathcal{F}_{\mathrm{qm}}$ and $\mathcal{F}_{\mathrm{FP}}$ is obvious, whereas for $\mathcal{K}_{\mathrm{qm}}$ and $\mathcal{K}_{\mathrm{FP}}$ we see that the operators $\Xi \mapsto [Q^n, \Xi]$ are replaced by directional derivatives $\xi \mapsto \boldsymbol{q}\cdot\nabla\xi$. Moreover the multiplication factor $u \geq 0$, which is the core of the Wasserstein theory, is replaced by the canonical correlation operator $\mathcal{C}_\rho \geq 0$, which also is homogeneous of degree 1 in the state variable ρ, i.e. $\mathcal{C}_{\lambda\rho} = \lambda\mathcal{C}_\rho$.

Finally, we consider Markov chains on a finite number of sites, namely $\{1, ..., N\}$. If p_n denotes the probability to be in site n, then the states $\boldsymbol{p} = (p_1, ..., p_N)^{\mathsf{T}}$ lie in the state space $\boldsymbol{X}_N = \{\, \boldsymbol{p} \in [0,1]^N \mid \boldsymbol{p}\cdot\boldsymbol{e} = 1 \,\}$, where $\boldsymbol{e} = (1, ..., 1)^{\mathsf{T}}$. The evolution is given in terms of the linear ODE

$$\dot{\boldsymbol{p}} = A\boldsymbol{p}, \quad \text{where } A \in \mathbb{R}^{N\times N} \text{ with } A_{ij} \geq 0 \text{ for } i \neq j \text{ and } A^{\mathsf{T}}\boldsymbol{e} = 0.$$

Here $A_{ij} \geq 0$ denotes the transition rate from j to i, and $A^{\mathsf{T}}\boldsymbol{e} = 0$ guarantees that $\boldsymbol{p}$ stays in $\boldsymbol{X}_N$.

We assume that the Markov chain $\dot{\boldsymbol{p}} = Q\boldsymbol{p}$ is irreducible, which means that the kernel of A is one-dimensional such that there is a unique steady state $\boldsymbol{w} = (w_1, ..., w_N)^{\mathsf{T}} \in \boldsymbol{X}_N$. An irreducible Markov chain is reversible (or is said to satisfy the 'condition of detailed balance'), if

$$A_{nm}w_m = A_{mn}w_n \quad \text{for all } n, m \in \{1, ..., N\}.$$

For such Markov chains $\dot{\boldsymbol{p}} = A\boldsymbol{p}$ it was shown in [Maa11, Mie11b] that they can be understood as the gradient system $(\boldsymbol{X}_N, \mathcal{F}_{\mathrm{Mv}}, \mathcal{K}_M K)$ with

$$\mathcal{F}_{\mathrm{Mv}}(\boldsymbol{p}) = \sum_{n=1}^{N} p_n \log(p_n/w_n) \quad \text{and}$$

$$\mathcal{K}_{\mathrm{Mv}}(\boldsymbol{p}) = \frac{1}{2}\sum_{n,m=1}^{N} A_{nm}w_m\Lambda\big(\tfrac{p_n}{w_n}, \tfrac{p_m}{w_m}\big)\,(\boldsymbol{e}^n - \boldsymbol{e}^m)\otimes(\boldsymbol{e}^n - \boldsymbol{e}^m) \in \mathbb{R}^{N\times N}_{\geq 0},$$

where Λ is defined in (4.3) and $\boldsymbol{e}^n$ denotes the n-th unit vector in $\mathbb{R}^N$. Note that $\mathcal{K}_{\mathrm{Mv}}$ again is homogeneous of degree 1, namely $\mathcal{K}_{\mathrm{Mv}}(\lambda \boldsymbol{p}) = \lambda \mathcal{K}_{\mathrm{Mv}}(\boldsymbol{p})$.

In fact, one can see the Markov chain as the restriction of the quantum mechanical density functional theory to the case that ρ is a diagonal matrix, i.e. $\rho = \mathrm{diag}(\boldsymbol{p}) \in \mathfrak{R}$. Thus, we restrict the non-commutative operator theory in $\mathrm{L}^2_{\mathrm{S}}(\mathbb{C}^N)$ to the commutative case in $\boldsymbol{X}_N$. Note that the dual dissipation potential Ψ^*_{Mv} can be rewritten using the canonical correlation operator and commutators as follows:

$$\Psi^*_{\mathrm{Mv}}(\boldsymbol{p}, \boldsymbol{\pi}) = \tfrac{1}{2}\boldsymbol{\pi} \cdot \mathcal{K}_{\mathrm{Mv}}(\boldsymbol{p})\boldsymbol{\pi} = \tfrac{1}{2}\sum_{n,m=1}^N \| [Q_{nm}, \mathrm{diag}(\boldsymbol{\pi})] \|^2_{\widehat{\mathcal{C}}_{\widehat{\rho}(\boldsymbol{p})}},$$

where $\widehat{\rho}(\boldsymbol{p}) = \mathrm{diag}(p_n/w_n)$ and $Q_{nm} = (A_{nm}w_m)^{1/2}\frac{1}{2}(\boldsymbol{e}^n \otimes \boldsymbol{e}^m + \boldsymbol{e}^m \otimes \boldsymbol{e}^n)$. This form shows clearly the analogy between reversible Markov chains and dissipative quantum mechanics.

Open problem 6: *It would be interesting to find sets of commutators $(Q^n)_{n=1,..,N}$ such that the distance $d_{\mathcal{K}_{\mathrm{qm}}}$ can be characterized in more detail. In particular, one would be interested in an explicit characterization like for the Wasserstein distance $d_{\mathcal{K}_{\mathrm{FP}}}$.*

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References

[AbM78] R. ABRAHAM and J. E. MARSDEN. *Foundations of mechanics*. Benjamin/Cummings Publishing Co. Inc. Advanced Book Program, Reading, Mass., 1978. Second edition, revised and enlarged, With the assistance of Tudor Raţiu and Richard Cushman.

[BhH88] R. BHATIA and J. A. R. HOLBROOK. On the Clarkson-McCarthy inequalities. *Math. Ann.*, 281(1), 7–12, 1988.

[GoK69] I. C. GOHBERG and M. G. KREIN. *Introduction to the theory of linear nonself-adjoint operators*. AMS Transl. Mathem. Monographs, 1969.

[Gra82] H. GRABERT. Nonlinear relaxation and fluctuations of damped quantum systems. *Z. Phys. B*, 49(2), 161–172, 1982.

[Grm10] M. GRMELA. Why GENERIC? *J. Non-Newtonian Fluid Mech.*, 165, 980–986, 2010.

[GrÖ97] M. GRMELA and H. C. ÖTTINGER. Dynamics and thermodynamics of complex fluids. I. Development of a general formalism. *Phys. Rev. E (3)*, 56(6), 6620–6632, 1997.

[HiS74] M. W. HIRSCH and S. SMALE. *Differential equations, dynamical systems, and linear algebra*. Academic Press, New York-London, 1974.

[JHÖ06] A. JELIĆ, M. HÜTTER, and H. C. ÖTTINGER. Dissipative electromagnetism from a nonequilibrium thermodynamics perspective. *Phys. Review E*, 74, 041126, 8 pp, 2006.

[JKO98] R. JORDAN, D. KINDERLEHRER, and F. OTTO. The variational formulation of the Fokker-Planck equation. *SIAM J. Math. Analysis*, 29(1), 1–17, 1998.

[KTH91] R. KUBO, M. TODA, and N. HASHITSUME. *Nonequilibrium Statistical Mechanics*. Springer, 2nd edition, 1991.

[Kub66] R. KUBO. The fluctuation-dissipation theorem. Part I. *Rep. Prog. Phys.*, 29, 255–284, 1966.

[LiM12] M. LIERO and A. MIELKE. Gradient structures and geodesic convexity for reaction-diffusion systems. *Phil. Trans. Royal Soc. A*, 2012. Submitted.

[Lin76] G. LINDBLAD. On the generators of quantum dynamical semigroups. *Comm. Math. Phys.*, 48(2), 119–130, 1976.

[Lin83] G. LINDBLAD. *Nonequilibrium entropy and irreversibility*, volume 5. D. Reidel Publishing Co., Dordrecht, 1983.

[Maa11] J. MAAS. Gradient flows of the entropy for finite Markov chains. *J. Funct. Anal.*, 261, 2250–2292, 2011.

[MaR99] J. E. MARSDEN and T. S. RATIU. *Introduction to Mechanics and Symmetry*, volume 17 of *Texts in Applied Mathematics*. Springer-Verlag, New York, second edition, 1999.

[Mie11a] A. MIELKE. Formulation of thermoelastic dissipative material behavior using GENERIC. *Contin. Mech. Thermodyn.*, 23(3), 233–256, 2011.

[Mie11b] A. MIELKE. Geodesic convexity of the relative entropy in reversible Markov chains. *Calc. Var. Part. Diff. Eqns.*, 2011. Submitted. WIAS preprint 1650.

[MiN12] A. MIELKE and H. NEIDHARDT. Coupling thermodynamics and quantum mechanics using generic. *In preparation*, 2012.

[MPA00] P. W. MICHOR, D. PETZ, and A. ANDAI. On the curvature of a certain Riemannian space of matrices. *Infin. Dimens. Anal. Quantum Probab. Relat. Top.*, 3(2), 199–212, 2000.

[ÖtG97] H. C. ÖTTINGER and M. GRMELA. Dynamics and thermodynamics of complex fluids. II. Illustrations of a general formalism. *Phys. Rev. E (3)*, 56(6), 6633–6655, 1997.

[Ott01] F. OTTO. The geometry of dissipative evolution equations: the porous medium equation. *Comm. Partial Differential Equations*, 26, 101–174, 2001.

[Ött05] H. C. ÖTTINGER. *Beyond Equilibrium Thermodynamics*. John Wiley, New Jersey, 2005.

[Ött10] H. C. ÖTTINGER. The nonlinear thermodynamic quantum master equation. *Phys. Rev. A*, 82, 052119(11), 2010.

[Ött11] H. C. ÖTTINGER. The geometry and thermodynamics of dissipative quantum systems. *Europhys. Lett.*, 94, 10006(6), 2011.

[PeS99] D. PETZ and C. SUDÁR. Extending the Fisher metric to density matrices. In O. Barndorff-Nielsen and E. Vendel Jensen, editors, *Geometry in Present Day Science*, pages 21–34. World Scientific, 1999.

[Pet94] D. PETZ. Geometry of canonical correlation on the state space of a quantum system. *J. Math. Phys.*, 35(2), 780–795, 1994.

[Str96] R. F. STREATER. Information geormetry and reduced quantum description. *Rep. Mathem. Physics*, 38, 419–436, 1996.

[Str00] R. F. STREATER. The analytic quantum information manifold. *Canadian Math. Soc. Conf. Proc.*, 29, 603–611, 2000.