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An entropic gradient structure for Lindblad equations and couplings of quantum systems to macroscopic models

Markus Mittnenzweig, Alexander Mielke

Abstract

We show that all Lindblad operators (i.e. generators of quantum semigroups) on a finite-dimensional Hilbert space satisfying the detailed balance condition with respect to the thermal equilibrium state can be written as a gradient system with respect to the relative entropy. We discuss also thermodynamically consistent couplings to macroscopic systems, either as damped Hamiltonian systems with constant temperature or as GENERIC systems. In particular, we discuss a model of a quantum dot coupled to macroscopic charge carriers.

1 Introduction

In many situations the evolution of quantum systems is dictated not only by the system Hamiltonian but also by dissipative effects, i.e. the time-dependent density matrix $\rho(t)$ satisfies a dissipative evolution equation of the form

$$\dot\rho = \frac{\mathrm{i}}{\hbar}\,\big[\rho, H\big]\; + \mathcal{L}\rho, \tag{1.1}$$

where we will set $\hbar = 1$ in the sequel. The dissipative part $\mathcal{L}$ of this Lindblad equation has to be the generator of semigroup consisting of completely positive operators, which is enforced by the structure of quantum mechanics. In this work we additionally ask for the ***condition of detailed balance*** with respect to the equilibrium state $\widehat\rho_\beta$ in the sense of Alicki [Ali76] and [KF*77], by which we mean that $\mathcal{L}\widehat\rho_\beta = 0$ and that $\mathcal{L}^*$ is symmetric with respect to the weighted operator scalar product $(A, B) \mapsto \mathrm{Tr}(A^*B\widehat\rho_\beta)$, see (2.4). We call such $\mathcal{L}$ shortly DBC Lindbladians with respect to $\widehat\rho_\beta$. Equations like (1.1) where already derived in the seminal work [Dav74] as the weak coupling limit of a given quantum system with a large heat bath. It was observed in [Spo78] that this class of models satisfies the detailed-balance condition (DBC) and that the relative entropy (also called free energy)

$$\mathcal{F}(\rho) = \mathrm{Tr}\,\big(\rho\,(\log\rho - \log\widehat\rho_\beta)\big) = \mathrm{Tr}\,\big(\rho\,(\log\rho + \beta H)\big) + \log Z_\beta$$

is a Liapunov function, i.e. it decays along solutions. Here $\beta > 0$ is a suitable inverse temperature and

$$\widehat\rho_\beta = \frac{1}{Z_\beta}\,\mathrm{e}^{-\beta H} \quad \text{with } Z_\beta = \mathrm{Tr}\,\big(\mathrm{e}^{-\beta H}\big)$$

is the thermal equilibrium.

The aim of this work is to show that (1.1) can be written as a damped Hamiltonian system, namely

$$\dot\rho = \big(\mathbb{J}(\rho) - \mathbb{K}(\rho)\big)\mathrm{D}\mathcal{F}(\rho), \tag{1.2}$$

where the operator $\mathbb{J}(\rho) : \xi \mapsto \frac{\mathrm{i}}{\beta}[\rho, \xi]$ generates a Poisson bracket, while the operator $\mathbb{K}(\rho)$ should be purely dissipative, i.e. $\mathbb{K}(\rho) = \mathbb{K}(\rho)^* \geq 0$. We will call such dissipative operators simply ***Onsager operators***, because of Onsager's fundamental work in [Ons31]. We continue to use D for the differential of functionals, i.e. $\langle \mathrm{D}\mathcal{F}(\rho), v\rangle := \lim_{h\to 0} \frac{1}{h}\big(\mathcal{F}(\rho{+}hv) - \mathcal{F}(\rho)\big)$.

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Thus, our aim is the construction of an Onsager operator $\mathbb{K}$ which generalizes the Wasserstein operator $\mathbb{K}_{\mathsf{Wass}}(u) : \mu \mapsto -\operatorname{div}\big(\rho\nabla\mu\big)$ for the Fokker-Planck equation and the Markov operator $\mathbb{K}_{\mathsf{Mv}}(p)$ for jump processes constructed in [Mie11b, Maa11, ErM12, Mie13b], cf. Section 3.1. The crucial point is that $\mathbb{K}(\rho)$ has to depend on ρ in a very specific way to obtain the relation

$$-\mathbb{K}(\rho)\big(\log\rho + \beta H\big) = \mathcal{L}\rho,$$

where the right-hand side is linear in ρ. In the Fokker-Plank equation this is achieved by the chain rule $u\nabla\big(\log u{+}V\big) = \nabla u{+}u\nabla V$, and for jump processes it follows from $\Lambda(a,b)(\log a{-}\log b) = a{-}b$, see Section 3.1.

For quantum systems first steps in this direction were done in [Ött10, Ött11, Mie13a, CaM14, Mie15]. They involve the use of the Kubo-Mori operator

$$\mathcal{C}_\rho : L(\mathfrak{h}) \to L(\mathfrak{h}); \quad A \mapsto \mathcal{C}_\rho A := \int_0^1 \rho^s\, A\, \rho^{1-s}\,\mathrm{d}s,$$

which satisfies for all $Q \in L(\mathfrak{h})$ the fundamental relation

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

which we will call the miracle relation. It goes back to [Kub59, Eqn. (2.17), p. 139] and was put into a more general context in [Wil67], see (2.5) there. Obviously, we need a generalization allowing for commutators of the form $[Q,\log\rho+\beta H]$, which is nontrivial if $\beta H \neq \alpha\mathbf{1}_{\mathfrak{h}}$. In [CaM14] the infinite-temperature case $\beta H = 0$ is treated, while in [Ött10, Ött11, Mie13a, Mie15] the nonlinear terms $\rho \mapsto \mathcal{C}_\rho[Q,H]$ are admitted.

Here, we show that in the general case with DBC it is possible to find a suitable $\mathbb{K}$ in a rather natural way. The starting point is a tensor-product representation of Lindblad operators. We set $\mathfrak{h}_1 = \mathfrak{h}$ and choose an arbitrary second Hilbert space $\mathfrak{h}_2$ and assume that $\mathfrak{h}_1$ and $\mathfrak{h}_2$ are finite-dimensional. For an arbitrary Hermitian $\mathbb{Q} \in L(\mathfrak{h}_1{\otimes}\mathfrak{h}_2)$ and a $\widehat\sigma \in L(\mathfrak{h}_2)$ with $\widehat\sigma = \widehat\sigma^* > 0$ one sees that

$$\mathcal{L}\rho = -\operatorname{Tr}_{\mathfrak{h}_2}\Big(\big[\mathbb{Q},[\mathbb{Q},\rho{\otimes}\widehat\sigma]\big]\Big) \tag{1.4}$$

is indeed a Lindblad operator. Moreover, it can be shown easily that this $\mathcal{L}$ satisfies the DBC with respect to $\widehat\rho_\beta$ if the commutation relation

$$\big[\,\mathbb{Q}\,,\,\widehat\rho_\beta\otimes\widehat\sigma\,\big] \;=\; 0$$

holds, see Section 2.3. Under this condition it is now straightforward to show the following generalization of the miracle identity:

$$\mathcal{C}_{\rho\otimes\widehat\sigma}\big[\,\mathbb{Q}\,,\,(\log\rho{+}\beta H)\otimes\mathbf{1}_{\mathfrak{h}_2}\,\big] = \big[\,\mathbb{Q}\,,\,\rho\otimes\widehat\sigma\,\big].$$

Indeed, it suffices to use the fact that $\mathbb{Q}$ also commutes with $\log(\widehat\rho_\beta{\otimes}\widehat\sigma) = -\beta H{\otimes}\mathbf{1}_{\mathfrak{h}_2} + \mathbf{1}_{\mathfrak{h}_1}{\otimes}\log\widehat\sigma$ and then apply the classical miracle identity (1.3), see Theorem 3.4 for the details. Now we can define the Onsager operator

$$\mathbb{K}(\rho)\xi = \operatorname{Tr}_{\mathfrak{h}_2}\Big(\big[\mathbb{Q},\mathcal{C}_{\rho\otimes\widehat\sigma}[\mathbb{Q},\xi{\otimes}\mathbf{1}_{\mathfrak{h}_2}]\big]\Big), \tag{1.5}$$

which is a symmetric and positive semidefinite operator and satisfies the desired relation

$$-\mathbb{K}(\rho)\big(\log\rho + \beta H\big) = -\operatorname{Tr}_{\mathfrak{h}_2}\Big(\big[\mathbb{Q},[\mathbb{Q},\rho{\otimes}\widehat\sigma]\big]\Big) = \mathcal{L}\rho, \tag{1.6}$$

which provides the entropic gradient structure for the dissipative terms. Thus,there is a full analogy to classical Markov processes, for which it was shown in [MPR14] that the DBC implies the existence of an entropic gradient structure.

In Theorem 2.7 we show that every DBC Lindbladian with respect to $\widehat{\rho}_\beta$ can be written in the form (1.4) with $\mathfrak{h}_2 = \mathfrak{h} = \mathfrak{h}_1$ and either $\widehat{\sigma} = \widehat{\rho}_\beta$ or $\widehat{\sigma} = \widehat{\rho}_\beta^{-1}$. Here we rely on the classical characterization of DBC Lindblad operators in [Ali76, KF*77].

In Sections 4 and 5 we consider a few applications and discuss the general problem of modeling the interaction of a macroscopic system described by a state variable $z \in Z$. We show that it is possible to set up a coupled system in the framework of GENERIC, which is an acronym for "General Equations for Non-Equilibrium Reversible and Irreversible Coupling". This framework is based on an energy functional $\mathcal{E}$, an entropy functional $\mathcal{S}$, a Poisson operator $\mathbb{J}$, and an Onsager operator $\mathbb{K}$ such that the evolution is

$$\begin{pmatrix}\dot\rho\\ \dot z\end{pmatrix} = \mathbb{J}_{\mathsf{coupl}}(\rho,z)\begin{pmatrix}\mathrm{D}_\rho\mathcal{E}(\rho,z)\\ \mathrm{D}_z\mathcal{E}(\rho,z)\end{pmatrix} + \mathbb{K}_{\mathsf{coupl}}(\rho,z)\begin{pmatrix}\mathrm{D}_\rho\mathcal{S}(\rho,z)\\ \mathrm{D}_z\mathcal{S}(\rho,z)\end{pmatrix}.$$

This is complemented by the fundamental ***non-interaction conditions*** $\mathbb{J}\mathrm{D}\mathcal{S} \equiv 0 \equiv \mathbb{K}\mathrm{D}\mathcal{E}$ that defines a thermodynamically consistent system with energy conservation and entropy production. The typical choice for the functionals is

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

To describe the coupling of the quantum system with the variable z it is essential to model the different dissipation mechanisms separately, which we do by the minimal building blocks $\mathcal{S}_W$ and $\mathcal{M}_Q^\beta$ for Lindblad operators, where Q must satisfy $[Q,H] = \omega Q$ for some $\omega \in \mathbb{R}$. The associated Onsager operators $\mathcal{K}_Q^\beta$ can then be obtained from the construction (1.5) by choosing

$$\mathbb{Q} = Q^* \otimes \begin{pmatrix}0&1\\0&0\end{pmatrix} + Q\otimes\begin{pmatrix}0&0\\1&0\end{pmatrix} \quad \text{and} \quad \widehat{\sigma} = \begin{pmatrix}\mathrm{e}^{\beta\omega/2}&0\\0&\mathrm{e}^{-\beta\omega/2}\end{pmatrix}.$$

With the above choice for $\mathcal{E}$ we have $\mathrm{D}_\rho\mathcal{E}(\rho,z) = H$, which forces us to use fixed eigenpairs (ω,Q). However, we may assume that the effective coupling temperature may depend on z and may differ for different coupling mechanisms. Hence, a typical Onsager operator for the coupling between a quantum system for ρ and a classical system for $z \in Z$ may have the form

$$\mathbb{K}_{\mathsf{coupl}}(\rho,z) = \sum_{m=1}^M \begin{pmatrix} \mathcal{K}_{Q_m}^{\widetilde\beta_m(z)}(\rho) & \langle\Box, b_m(z)\rangle_Z \mathcal{K}_{Q_m}^{\widetilde\beta_m(z)}(\rho)H \\ \langle\!\langle \mathcal{K}_{Q_m}^{\widetilde\beta_m(z)}(\rho)\Box \,\|\, H\rangle\!\rangle b_m(z) & \langle\!\langle \mathcal{K}_{Q_m}^{\widetilde\beta_m(z)}(\rho)H \,\|\, H\rangle\!\rangle b_m(z)\otimes b_m(z)\end{pmatrix},$$

where $\langle\cdot,\cdot\rangle_Z$ denotes the dual pairing between Z^* and Z, while $\langle\!\langle\, A \,\|\, B \,\rangle\!\rangle$ denotes the (Hilbert-Schmidt) scalar product $\mathrm{Tr}(A^*B)$ for operators, see Section 2.1. For an application to the thermodynamically consistent modeling of the Maxwell-Bloch system as considered in [JMR00, Dum05] we refer to Section 5.5, where the macroscopical variable $z = (\boldsymbol{E},\boldsymbol{H})$ contains the electric and the magnetic field. For more applications, also involving the coupling to drift-diffusion equations we refer to [Mie15, Sec. 5].

For the sake of notational simplicity and to avoid technical complications, we have restricted ourselves to the finite-dimensional case $\dim\mathfrak{h} < \infty$. Many results have an immediate generalization to the infinite-dimensional case, e.g. the relations (1.3) to (1.6). However, the full characterization of all DBC

Lindbladians, which is given in Theorem 2.7 or Proposition 2.2, would require much more delicate considerations and thus remains an open question.

Note added in proof: After this work was finished the authors became aware of the parallel and totally independent work [CaM16], which has some overlap concerning the construction of an entropic gradient structure for Lindblad equations with detailed balance.

2 Dissipative quantum mechanics

2.1 General notations and setup

Here we recall the standard theory and introduce our notation. The quantum mechanical system is described by states in a complex Hilbert space $\mathfrak{h}$ with scalar product $\langle a|b\rangle$. For a Hamiltonian operator $H \in \mathrm{Herm}(\mathfrak{h})$ (the set of Hermitian operators on $\mathfrak{h}$) the associated Hamiltonian dynamics is given via the Schrödinger equation $\dot{\psi} = -\mathrm{i}H\psi$, which has the solution $\psi(t) = \mathrm{e}^{-\mathrm{i}tH}\psi(0)$.

To couple a quantum system to a macroscopic one we need to describe it in statistical terms using the density matrices

$$\rho \in \mathfrak{R}_N := \{\, \rho \in L(\mathfrak{h}) \mid \rho = \rho^* \geq 0,\ \mathrm{Tr}\ \rho = 1 \,\}.$$

Each $\rho \in \mathfrak{R}_N$ has the representation

$$\rho = \sum_{j=1}^{N} r_j \,|\psi_j\rangle\,\langle\psi_j|, \tag{2.1}$$

where $r_j \geq 0$, $\sum_1^N r_j = 1$, and $\{\, \psi_j \mid j = 1, ..., N \,\}$ is an orthonormal set. Note that in our notation $(|\psi\rangle\,\langle\phi|)\, a := \langle\phi|a\rangle\psi$ and $(|\psi\rangle\,\langle\phi|)A = |\psi\rangle\,\langle A^*\phi|$.

On operators we define the Hilbert-Schmidt scalar product $\langle\!\langle\, A \,\|\, B \,\rangle\!\rangle = \mathrm{Tr}(A^*B)$ satisfying the following identities, which will be used below without further notice:

$$\langle\!\langle A \| B \rangle\!\rangle = \langle\!\langle B^* \| A^* \rangle\!\rangle = \overline{\langle\!\langle B \| A \rangle\!\rangle}, \qquad \langle\!\langle \lambda A \| \mu B \rangle\!\rangle = \overline{\lambda}\mu\langle\!\langle A \| B \rangle\!\rangle,$$
$$\langle\!\langle A \| BC \rangle\!\rangle = \langle\!\langle AC^* \| B \rangle\!\rangle = \langle\!\langle B^*A \| C \rangle\!\rangle, \quad \langle\!\langle A \| [B,C] \rangle\!\rangle = \langle\!\langle B^* \| [C,A^*] \rangle\!\rangle = \langle\!\langle C^* \| [A^*,B] \rangle\!\rangle,$$

where $\lambda, \mu \in \mathbb{C}$ and $A, B, C \in L(\mathfrak{h})$.

2.2 The Lindblad equations

Using the Schrödinger equation the evolution of ρ is given via the Liouville-von Neumann equation

$$\dot{\rho} = -\mathrm{i}[H,\rho], \quad \text{where } [\rho, H] := \rho H - H\rho. \tag{2.2}$$

For open systems, dissipative versions of the Hamiltonian Liouville–von Neumann equation are used. The most general linear master equation preserving complete positivity is the well-known Lindblad equation

$$\dot{\rho} = -\mathrm{i}[H,\rho] + \mathcal{L}\rho \quad \text{with } \mathcal{L}A = \sum_{n,m=1}^{N^2-1} a_{n,m}\big([Q_n, AQ_m^*] + [Q_nA, Q_m^*]\big), \tag{2.3}$$

where Q_n are arbitrary operators in $L(\mathfrak{h}) := \mathrm{Lin}(\mathfrak{h},\mathfrak{h})$, and $(a_{n,m})$ is a Hermitian positive semi-definite matrix. Note that $\mathcal{L}$ in the Lindblad equation is evaluated only on $\rho \in \mathfrak{R}$, while we prefer to define $\mathcal{L}$ as an operator mapping from all of $L(\mathfrak{h})$ into $L(\mathfrak{h})$. It is easily seen that every $\mathcal{L}$ is a $*$-operator, i.e. it satisfies $\mathcal{L}(A^*) = (\mathcal{L}\mathcal{A})^*$. The set of all Lindblad operators forms a cone of real dimension $(N^2{-}1)^2$ in the set of linear operators from $L(\mathfrak{h})$ into itself. Characterizing the steady states and the dynamics of a general Lindblad operator remains a field of ongoing research [BNT08, BaN08, BaN12].

In this work we are mainly interested in Lindblad operators satisfying the detailed balance condition (DBC), shortly called DBC Lindbladians. We follow the definition in [Ali76, KF*77] and refer to [AJ*06] for a discussion of other versions of the DBC. Let $\mathcal{L}^*$ denote the adjoint of $\mathcal{L}$ defined via $\langle\!\langle\, \mathcal{L}^* A \,\|\, B \,\rangle\!\rangle = \langle\!\langle\, A \,\|\, \mathcal{L}B \,\rangle\!\rangle$. The ***condition of detailed balance*** with respect to the equilibrium state $\widehat\rho_\beta$ is defined via the relation

$$\text{(DBC)} \qquad \begin{cases} \mathcal{L}\widehat\rho_\beta = 0, \\ \langle\!\langle\, \mathcal{L}^*(A) \,\|\, B\widehat\rho_\beta \,\rangle\!\rangle = \langle\!\langle\, A \,\|\, \mathcal{L}^*(B)\widehat\rho_\beta \,\rangle\!\rangle \quad \text{for all } A,B \in L(\mathfrak{h}), \end{cases} \tag{2.4}$$

i.e. $\mathcal{L}^*$ is symmetric with respect to the weighted scalar product $(A,B) \mapsto \langle\!\langle\, A \,\|\, B\widehat\rho_\beta \,\rangle\!\rangle$. The characterization of all operators lying in the class of DBC Lindbladians for a fixed $\widehat\rho_\beta$ is given in [Ali76, Eqn. (20)]. See also [JPW14] for a modern characterization of DBC Lindblad operators, while there the main goal is a large deviations theory for the asymptotics for $t \to \infty$. We will derive a new and compact representation of these operators in Section 2.3. Clearly, the DBC is equivalent to

$$\mathcal{L}(A\widehat\rho_\beta) = \mathcal{L}^*(A)\widehat\rho_\beta \quad \text{for all } A \in L(\mathfrak{h}). \tag{2.5}$$

Before discussing the general form of ***all*** DBC Lindbladians, we will construct minimal building blocks. They are useful in their own right for the modeling of dissipative couplings as discussed in Sections 4 and 5. The main observation is that the property of detailed balance with respect to $\widehat\rho_\beta = \frac{1}{Z_\beta}\mathrm{e}^{-\beta H}$ involves operators Q having the property $\widehat\rho_\beta Q(\widehat\rho_\beta)^{-1} = \mu Q$, which can be characterized by the following elementary result.

Lemma 2.1 *For $\omega \in \mathbb{R}$, $H \in \mathrm{Herm}(\mathfrak{h})$ and $Q \in L(\mathfrak{h})$ we have the equivalences:*

$$\begin{aligned} \textit{(i)}\ [Q,H] = \omega Q \quad &\Longleftrightarrow \quad \textit{(ii)}\ \exists\, \beta \neq 0 :\ \mathrm{e}^{-\beta H} Q \mathrm{e}^{\beta H} = \mathrm{e}^{\beta\omega} Q \\ &\Longleftrightarrow \quad \textit{(iii)}\ \forall\, \gamma \in \mathbb{R} :\ \mathrm{e}^{-\gamma H} Q \mathrm{e}^{\gamma H} = \mathrm{e}^{\gamma\omega} Q. \end{aligned} \tag{2.6}$$

We note that operators with the commutator property (i) can easily be constructed when using the spectral representation of the Hamiltonian H, namely

$$H = \sum_{n=1}^{N} \varepsilon_n |h_n\rangle\,\langle h_n|, \quad \text{and hence } \widehat\rho_\beta = \frac{1}{Z_\beta}\sum_{n=1}^{N} \mathrm{e}^{-\beta\varepsilon_n}|h_n\rangle\,\langle h_n| \text{ with } Z_\beta = \sum_{n=1}^{N}\mathrm{e}^{-\beta\varepsilon_n}.$$

For a given eigenvalue ε_n we define the spectral projector P_n via

$$P_n = \sum_{k:\varepsilon_k=\varepsilon_n} |h_k\rangle\,\langle h_k|, \quad \text{giving } P_n = P_n^2 = P_n^* \text{ and } P_nH = HP_n = \varepsilon_n P_n.$$

Now we can take any operator $V \in L(\mathfrak{h})$ and choose spectral projectors P_n and P_m. Then

$$Q = P_nVP_m \quad \text{satisfies} \quad [Q,H] = (\varepsilon_m{-}\varepsilon_n)Q.$$

We emphasize that this relation is linear in Q, so that a general Q satisfying $[Q,H]=\omega Q$ may have the form

$$Q=\sum_{(n,m):\,\varepsilon_m-\varepsilon_n=\omega} P_n V_{n,m} P_m,$$

thus possibly more than two energy levels ε_k may be involved. This is trivial for the case $\omega=0$ but may also occur in the case $\omega\neq 0$, see Example 2.4.2.

We introduce the spectrum $\Omega(H)$ of the map $A\mapsto[A,H]$ and the set $\mathfrak{E}(H)$ of eigenpairs via

$$\begin{aligned}\Omega(H) &:= \mathrm{spec}([\,\cdot\,,H]) = \big\{\,\varepsilon_m-\varepsilon_n\,\big|\,\varepsilon_n,\varepsilon_m\in \mathsf{spec}(H)\,\big\},\\ \mathfrak{E}(H) &:= \big\{\,(\omega,Q)\in\mathbb{R}\times L(\mathfrak{h})\,\big|\,[Q,H]=\omega Q\,\big\}.\end{aligned}$$

Let us further define the multiplicities of the eigenspaces via

$$d_\omega=\mathsf{dim}\big\{\,Q\in L(\mathfrak{h})\,\big|\,[Q,H]=\omega Q\,\big\}.$$

If H has only one-dimensional eigenspaces and no pairs of eigenvalues $\varepsilon_m,\varepsilon_n$ ($m\neq n$) have equal differences $\varepsilon_m-\varepsilon_n=\varepsilon_{m'}-\varepsilon_{m'}$, then $d_\omega=1$ for $\omega\neq 0$ and $d_0=N$. However, in the most degenerate case $H=0$ we find $d_0=N^2$ and $d_\omega=0$ for all ω. The following result provides the building blocks for all DBC Lindbladians with respect to $\widehat{\rho}_\beta=\frac{1}{Z_\beta}\mathrm{e}^{-\beta H}$.

Proposition 2.2 (Building blocks $\mathcal{S}_W$ and $\mathcal{M}_Q^\beta$) *Let H and $\widehat{\rho}_\beta$ be given as above.*

(a) Consider any $W\in\mathrm{Herm}(\mathfrak{h})$ with $[W,H]=0$, then the operator $\mathcal{S}_W$ defined by

$$\mathcal{S}_W A \;:=\; [W,AW]+[WA,W]=\big[W,[A,W]\big]$$

is a Lindblad operator satisfying $\mathcal{S}_W=\mathcal{S}_W^*$ and the DBC for $\widehat{\rho}_\beta$.

(b) Consider any pair $(\omega,Q)\in\mathfrak{E}(H)$, then the operator $\mathcal{M}_Q^\beta$ defined via

$$\mathcal{M}_Q^\beta A \;:=\; \mathrm{e}^{\beta\omega/2}\big([Q,AQ^*]+[QA,Q^*]\big)+\mathrm{e}^{-\beta\omega/2}\big([Q^*,AQ]+[Q^*A,Q]\big)$$

is a DBC Lindbladian for $\widehat{\rho}_\beta$.

(c) Every Lindbladian $\mathcal{L}$ satisfying the DBC (2.4) *can be written in the form*

$$\mathcal{L}=\sum_{j=1}^{J}\mathcal{S}_{W_j}+\sum_{m=1}^{M}\mathcal{M}_{Q_m}^\beta,\quad \textit{where}\;\begin{cases} W_j=W_j^*,\ (0,W_j)\in\mathfrak{E}(H),\ \textit{and}\\ (\omega_m,Q_m)\in\mathfrak{E}(H)\ \textit{with}\ \omega_m>0.\end{cases}$$

The numbers J and M of necessary terms is bounded by $J\leq d_0-1$ and $M\leq\sum_{\omega\in\Omega(H)\setminus\{0\}}d_\omega$.

Proof: Part (a): Obviously, $\mathcal{S}_W$ is a special case of $\mathcal{L}$ in (2.3) by choosing $a_{1,1}=1$ and $Q_1=W$ and $a_{n,m}=0$ for $(n,m)\neq(1,1)$, so it is a Lindblad operator. We also see that the DBC $\mathcal{S}_W^{\widehat{\rho}_\beta}=\mathcal{S}_W$ holds, since $\widehat{\rho}_\beta W\widehat{\rho}_\beta^{-1}=W$ by using Lemma 2.1.

Part (b): It is obvious that $\mathcal{M}_Q^\beta$ has the form of $\mathcal{L}$ in (2.3) with $Q_1=Q$, $Q_2=Q^*$, $a_{1,1}=\mathrm{e}^{\beta\omega/2}$, and $a_{2,2}=\mathrm{e}^{-\beta\omega/2}$, while all other terms are 0. Moreover, $\Big(\mathcal{M}_Q^\beta\Big)^{\widehat{\rho}_\beta}$ can be calculated explicitly by using Lemma 2.1 and $\widehat{\rho}_\beta Q^*\widehat{\rho}_\beta^{-1}=\mathrm{e}^{-\beta\omega}Q^*$, so the DBC follows.

Part (c): From [KF*77, Eqn. (2.16)-(2.20)] (where L_s corresponds to our $\mathcal{L}^*$) we know that every DBC Lindbladian with respect to $\widehat{\rho}_\beta$ can be written as

$$\mathcal{L}A = \sum_{k,j=1}^{N} D_{kj}\big([X_{kj}A, X_{kj}^*] + [X_{kj}, AX_{kj}^*]\big), \tag{2.7}$$

where $D_{kj} \geq 0$ and $X_{kj} \in \mathbb{C}^{N\times N}$ satisfy the conditions (with $\widehat{r}_j = \mathrm{e}^{-\beta\varepsilon_j}/Z_\beta > 0$)

$$\begin{aligned} &\text{(i) } D_{kj}\widehat{r}_j = D_{jk}\widehat{r}_k \text{ and } X_{kj}^* = X_{jk} \text{ for } \widehat{r}_j \neq \widehat{r}_k; \quad \text{(ii) } \langle\!\langle X_{kj} \,\|\, X_{lm} \rangle\!\rangle = \delta_{kl}\delta_{jm};\\ &\text{(iii) } X_{kj}^* = X_{kj} \text{ for } \widehat{r}_j = \widehat{r}_k; \quad \text{(iv) } \widehat{\rho}_\beta\, X_{kj}(\widehat{\rho}_\beta)^{-1} = \frac{\widehat{r}_k}{\widehat{r}_j}\, X_{kj}. \end{aligned} \tag{2.8}$$

We decompose the set $I = \{1,..,N\}^2$ into $I_{\neq} := \{\, (k,j) \in \{1,..,N\}^2 \mid \widetilde{r}_j \neq \widehat{r}_k \,\}$ and $I_= := \{\, (k,j) \in \{1,..,N\}^2 \mid \widetilde{r}_j = \widehat{r}_k \,\}$. For $(j,k) \in I_{\neq}$ the second condition in (i) gives $X_{jk} = X_{kj}^*$, while (iv) and Lemma 2.1 imply $(\varepsilon_k{-}\varepsilon_j, X_{kj}) \in \mathfrak{E}(H)$. Using now the first condition in (i) as well and setting $Q_{kj} = \mathrm{e}^{\beta(\varepsilon_k-\varepsilon_j)/4}X_{kj}$, we find the relation

$$D_{kj}\big([X_{kj}A, X_{kj}^*] + [X_{kj}, AX_{kj}^*]\big) + D_{jk}\big([X_{jk}A, X_{jk}^*] + [X_{jk}, AX_{jk}^*]\big) = \mathcal{M}^\beta_{Q_{kj}}A.$$

For $(k,j) \in I_=$ conditions (iii) and (iv) yield $X_{kj} = X_{kj}^*$ and $[X_{kj}, H] = 0$. Thus,

$$D_{kj}\big([X_{kj}A, X_{kj}^*] + [X_{kj}, AX_{kj}^*]\big) = \mathcal{S}_{W_{kj}}A \text{ with } W_{kj} = \sqrt{D_{kj}}X_{kj}.$$

In summary, we find that $\mathcal{L}$ in (2.7) can be written in the form

$$\mathcal{L} = \sum_{(k,j)\in I_=} \mathcal{S}_{W_{kj}} + \sum_{(k,j)\in I_{\neq},\, j<k} \mathcal{M}^\beta_{Q_{kj}},$$

which is the desired result. ■

Note that the representation of $\mathcal{L}$ in terms of the Kraus operators Q_n in (2.3) is not unique. Correspondingly, our representation in terms of $\mathcal{S}_{W_j}$ and $\mathcal{M}_{Q_j}$ is not unique. Moreover, for a minimal representation one may ask for additional orthogonality conditions. We also remark that the operators $\mathcal{S}_W$ can be obtained from $\mathcal{M}_Q$ as a special case allowing $\omega = 0$ and asking for $Q = Q^*$. More precisely, if $(0,Q) \in \mathfrak{E}(H)$ then also $(0,Q^*)$ and $(0, \frac{1}{2}(Q{+}Q^*))$ lie in $\mathfrak{E}(H)$. In particular, we have

$$(0,Q) \in \mathfrak{E}(H) \text{ and } Q = Q^* \quad \Longrightarrow \quad \mathcal{M}^\beta_Q = 2\mathcal{S}_{\beta,Q} = \mathcal{S}_{\beta,\sqrt{2}\,Q}.$$

Moreover, $(\omega,Q) \in \mathfrak{E}(H)$ if and only if $(-\omega,Q^*) \in \mathfrak{E}(H)$ and $\mathcal{M}^\beta_Q = \mathcal{M}^\beta_{Q^*}$. Thus, Proposition 2.2(c) tells us that all DBC Lindbladians can be written in the form

$$\mathcal{L}\rho = \sum_{n=1}^{N} \mathcal{M}^\beta_{Q_n}\rho \quad \text{where } (\omega_n, Q_n) \in \mathfrak{E}(H) \text{ and } \omega_j \in \Omega(H). \tag{2.9}$$

We will see specific examples in Sections 2.4 and 5. The above representation in terms of the building blocks is especially useful for modeling, while the next section provides a form that is more elegant and compact.

2.3 A compact form of all DBC Lindblad operators

In this section we will write Lindblad operators and our building blocks 2.2 in another way. The basic idea is to write them as the partial trace of a double commutator on a larger space. This will prove useful in Section 3 when writing down entropic gradient structures for the Lindblad equations with DBC. In what follows $\mathfrak{h}_1$ and $\mathfrak{h}_2$ denote finite-dimensional Hilbert spaces, and for $A \in L(\mathfrak{h}_1)$ and $B \in L(\mathfrak{h}_2)$ we denote the tensor product by $A \otimes B \in L(\mathfrak{h}_1) \otimes L(\mathfrak{h}_2) = L(\mathfrak{h}_1 \otimes \mathfrak{h}_2)$. We also introduce the notion of a partial trace

$$\mathrm{Tr}_{\mathfrak{h}_2} : L(\mathfrak{h}_1) \otimes L(\mathfrak{h}_2) \to L(\mathfrak{h}_1) \text{ defined via } \mathrm{Tr}_{\mathfrak{h}_2}(A \otimes B) = \mathrm{Tr}_2(B) A$$

on direct products and extended by linearity to the whole space $L(\mathfrak{h}_1 \otimes \mathfrak{h}_2)$. Here Tr_2 is the trace in $L(\mathfrak{h}_2)$.

The next result shows that all Lindblad operators on $L(\mathfrak{h}_1)$ can be written in a compact form by a double commutator on $L(\mathfrak{h}_1) \otimes L(\mathfrak{h}_2)$ and a partial trace. Moreover, this form allows for a simple criterion for the DBC with respect to the equilibrium $\widehat{\rho}_\beta$.

Proposition 2.3 (Compact representation for $\mathcal{L}$) *Consider two finite dimensional Hilbert spaces $\mathfrak{h}_1$ and $\mathfrak{h}_2$. Assume that $\mathbb{Q} \in \mathrm{Herm}(\mathfrak{h}_1 \otimes \mathfrak{h}_2)$, $\widehat{\sigma} \in \mathrm{Herm}(\mathfrak{h}_2)$ and $\widehat{\sigma} \geq 0$. Then*

$$\mathcal{L}(\rho) = -\,\mathrm{Tr}_{\mathfrak{h}_2}\Big(\big[\mathbb{Q}, [\mathbb{Q}, \rho \otimes \widehat{\sigma}]\big]\Big) \tag{2.10}$$

is a Lindblad operator in $L(\mathfrak{h}_1)$, i.e. the generator of a completely positive semigroup.

If in addition $\mathbb{Q}$ and $\widehat{\sigma}$ satisfy the commutator relation

$$\big[\mathbb{Q}, \widehat{\rho}_\beta \otimes \widehat{\sigma}\big] = 0, \tag{2.11}$$

then $\mathcal{L}$ satisfies the DBC with respect to $\widehat{\rho}_\beta$.

Proof: Since $\widehat{\sigma} \geq 0$ we can write $\widehat{\sigma} = \sum_{j=1}^J \sigma_j e_j \otimes \overline{e}_j$ with $\sigma_j \geq 0$. Let us define

$$Q_{kl} = \langle e_k \,|\mathbb{Q}|\, e_l \rangle_{\mathfrak{h}_2} = \mathrm{Tr}_{\mathfrak{h}_2}(\mathbf{1}_{\mathfrak{h}_1} \otimes (e_l \otimes \overline{e}_k)\mathbb{Q}) \text{ giving } \mathbb{Q} = \sum_{k,l} Q_{kl} \otimes (e_l \otimes \overline{e}_k).$$

Then $Q_{kl} = Q_{lk}^*$ and using $\mathrm{Tr}_{\mathfrak{h}_2}\big(B \otimes \big((e_k \otimes \overline{e}_l) \otimes (e_m \otimes \overline{e}_n)\big)\big) = \delta_{kn}\delta_{lm} B$ we find

$$\mathcal{L}\rho = \sum_{k,l=1}^J \big(2\sigma_l Q_{kl} \rho Q_{lk} - \sigma_k \{Q_{kl} Q_{lk}, \rho\}\big) = \sum_{k,l=1}^J \sigma_l \big([Q_{kl}\rho, Q_{kl}^*] + [Q_{kl}, \rho Q_{kl}^*]\big). \tag{2.12}$$

which is clearly of Lindblad form.

The commutation relation (2.11) immediately implies $\mathcal{L}\widehat{\rho}_\beta = 0$, which is the first relation in the DBC (2.4). The second relation is written in terms of the dual operator $\mathcal{L}^*$ that takes the form

$$\mathcal{L}^*(A) = \mathrm{Tr}_{\mathfrak{h}_2}(\mathbf{1}_{\mathfrak{h}_1} \otimes \widehat{\sigma}\ \big[\mathbb{Q}, \big[\mathbb{Q}, A \otimes \mathbf{1}_{\mathfrak{h}_2}\big]\big]).$$

We have to show $\mathrm{Tr}\,\big((\mathcal{L}^* A)^* B \widehat{\rho}_\beta)\big) = \mathrm{Tr}(A^* \mathcal{L}^*(B)\widehat{\rho}_\beta)$. Using $(\mathcal{L}^* A)^* = \mathcal{L}^*(A^*)$ the left hand side is equivalent to

$$\begin{aligned}\mathrm{Tr}_{\mathfrak{h}_1}(\mathcal{L}^*(A^*) B \widehat{\rho}_\beta) &= \mathrm{Tr}_{\mathfrak{h}_1 \otimes \mathfrak{h}_2}(\mathbf{1}_{\mathfrak{h}_1} \otimes \widehat{\sigma}\ \big[\mathbb{Q}, \big[\mathbb{Q}, A^* \otimes \mathbf{1}_{\mathfrak{h}_2}\big]\big]\ (B\widehat{\rho}_\beta) \otimes \mathbf{1}_{\mathfrak{h}_2}) \\ &= \mathrm{Tr}_{\mathfrak{h}_1 \otimes \mathfrak{h}_2}(\ \big[\mathbb{Q}, \big[\mathbb{Q}, A^* \otimes \mathbf{1}_{\mathfrak{h}_2}\big]\big]\ (B \otimes \mathbf{1}_{\mathfrak{h}_2}) \widehat{\rho}_\beta \otimes \widehat{\sigma}).\end{aligned}$$

Again using the commutator condition (2.11) we obtain, for all $\mathbb{A}$, the identity

$$[\mathbb{Q},\mathbb{A}(\widehat{\rho}_\beta\otimes\widehat{\sigma})] = +\,[\mathbb{Q},\mathbb{A}]\,\widehat{\rho}_\beta\otimes\widehat{\sigma} + \mathbb{A}\,[\mathbb{Q},\widehat{\rho}_\beta\otimes\widehat{\sigma}] = [\mathbb{Q},\mathbb{A}]\,\widehat{\rho}_\beta\otimes\widehat{\sigma},$$

which we use twice, namely once with $\mathbb{A} = B\otimes\mathbf{1}_{\mathfrak{h}_2}$ and once with $\mathbb{A} = \big[\mathbb{Q}, B\otimes\mathbf{1}_{\mathfrak{h}_2}\big]$. Thus, we can move the $\mathbb{Q}$ operators to the right and obtain

$$\begin{aligned}\mathrm{Tr}_{\mathfrak{h}_1}(\mathcal{L}^*(A^*)B\widehat{\rho}_\beta) &= \mathrm{Tr}_{\mathfrak{h}_1\otimes\mathfrak{h}_2}(A^*\otimes\mathbf{1}_{\mathfrak{h}_2}\ \big[\mathbb{Q},\big[\mathbb{Q},(B\otimes\mathbf{1}_{\mathfrak{h}_2})\big]\big]\,\widehat{\rho}_\beta\otimes\widehat{\sigma})\\ &= \mathrm{Tr}_{\mathfrak{h}_1}(A^*\mathrm{Tr}_{\mathfrak{h}_2}(\big[\mathbb{Q},\big[\mathbb{Q},(B\otimes\mathbf{1}_{\mathfrak{h}_2})\big]\big]\,\mathbf{1}\otimes\widehat{\sigma})\widehat{\rho}_\beta)\\ &= \mathrm{Tr}_{\mathfrak{h}_1}(A^*\mathcal{L}^*(B)\widehat{\rho}_\beta),\end{aligned}$$

which is the desired DBC. ■

The above result shows that the commutator relation (2.11) is crucial for the study of DBC Lindbladians. In the following lemma we give an alternative characterization which will be useful later, when studying the associated gradient structures.

Lemma 2.4 (Equivalent commutation relation) *Consider* $\mathbb{Q} \in \mathrm{Herm}(\mathfrak{h}_1\otimes\mathfrak{h}_2)$, $\widehat{\rho} \in \mathrm{Herm}(\mathfrak{h}_1)$, *and* $\widehat{\sigma} \in \mathrm{Herm}(\mathfrak{h}_2)$ *with* $\widehat{\rho},\widehat{\sigma} > 0$. *Then we have*

$$[\mathbb{Q},\widehat{\rho}\otimes\widehat{\sigma}] = 0 \quad\Longleftrightarrow\quad [\mathbb{Q},\log\widehat{\rho}\otimes\mathbf{1}_{\mathfrak{h}_2}] + [\mathbb{Q},\mathbf{1}_{\mathfrak{h}_1}\otimes\log\widehat{\sigma}] = 0. \tag{2.13}$$

Proof: We simply note that a Hermitian operator $\mathbb{Q}$ commutes with a Hermitian operator $\mathbb{B} > 0$ if and only if it commutes with its logarithm $\log\mathbb{B}$. We apply this to $\mathbb{B} = \widehat{\rho}\otimes\widehat{\sigma}$, for which we have

$$\log(\widehat{\rho}\otimes\widehat{\sigma}) = \log\widehat{\rho}\otimes\mathbf{1}_{\mathfrak{h}_2} \ +\ \mathbf{1}_{\mathfrak{h}_1}\otimes\log\widehat{\sigma}.$$

This gives the desired result. ■

The above proposition demonstrates that the definition (2.10) together with (2.11) generates DBC Lindbladians. The following corollary shows that the building blocks $\mathcal{S}_W$ and $\mathcal{M}_Q^\beta$ from Proposition 2.2 can be written in the compact form (2.10) as well.

Corollary 2.5 (Building blocks in compact form) *Consider* $\widehat{\rho}_\beta = \frac{1}{Z_\beta}\mathrm{e}^{-\beta H}$ *with* $H \in \mathrm{Herm}(\mathfrak{h}_1)$.

(1) Choosing $\mathfrak{h}_2 = \mathbb{C}$ *and* $\mathbb{Q}_W = W$ *for* $W \in \mathrm{Herm}(\mathfrak{h}_1)$ *we have the identity*

$$\mathcal{S}_W A = [W,AW] + [WA,W] = -\big[W,[W,A]\big] = -\big[\mathbb{Q}_W,[\mathbb{Q}_W,A]\big].$$

The commutator relation (2.13) *for* $\mathbb{Q}_W$ *is simply* $[H,W] = 0$.

(2) Choosing $\mathfrak{h}_2 = \mathbb{C}^2$ *and* $(\omega,Q) \in \mathfrak{E}(H)$ *we define*

$$\mathbb{Q}_Q = \begin{pmatrix} 0 & Q^* \\ Q & 0\end{pmatrix} \quad \widehat{\sigma}_{\beta\omega} = \begin{pmatrix} \mathrm{e}^{\beta\omega/2} & 0 \\ 0 & \mathrm{e}^{-\beta\omega/2}\end{pmatrix}.$$

Then, the commutation relation (2.13) *holds and we have*

$$\begin{aligned}\mathcal{M}_Q^\beta A &= -\,\mathrm{Tr}_{\mathfrak{h}_2}([\mathbb{Q}_Q,[\mathbb{Q}_Q,A\otimes\widehat{\sigma}_{\beta\omega}]])\\ &= \mathrm{e}^{\beta\omega/2}([Q,\rho Q^*] + [Q\rho,Q^*]) + \mathrm{e}^{-\beta\omega/2}([Q^*,\rho Q] + [Q^*\rho,Q]).\end{aligned} \tag{2.14}$$

Proof: (1) is trivial. For (2) the relation (2.14) follows from a direct calculation of the partial trace. In order to check the commutation condition (2.11) we observe

$$[\mathbb{Q}_Q, \widehat{\rho}_\beta \otimes \widehat{\sigma}_{\beta\omega}] = \begin{pmatrix} 0 & \mathrm{e}^{-\frac{\beta\omega}{2}} Q^* \widehat{\rho}_\beta - \mathrm{e}^{\frac{\beta\omega}{2}} \widehat{\rho}_\beta Q^* \\ \mathrm{e}^{\frac{\beta\omega}{2}} Q \widehat{\rho}_\beta - \mathrm{e}^{-\frac{\beta\omega}{2}} \widehat{\rho}_\beta Q & 0 \end{pmatrix}.$$

By Lemma 2.1 the relation $[Q, H] = \omega Q$ is equivalent to $\mathrm{e}^{\beta\omega/2} \widehat{\rho}_\beta Q = \mathrm{e}^{-\beta\omega/2} Q \widehat{\rho}_\beta$, so indeed the commutator $[\mathbb{Q}_Q, \widehat{\rho}_\beta \otimes \widehat{\sigma}_{\beta\omega}]$ vanishes. ∎

As a last step we want to show that all DBC Lindbladians can be written in the form (2.10) with a particular choice of $\widehat{\sigma}$, namely either $\widehat{\sigma} = \widehat{\rho}_\beta$ or $\widehat{\sigma} = \widehat{\rho}_\beta^{-1}$. Therefore, we introduce a ***partial transpose*** on $L(\mathfrak{h}_1 \otimes \mathfrak{h}_2)$ that acts on the $\mathfrak{h}_2$ part and is associated with a fixed $\widehat{\sigma} = \widehat{\sigma}^* > 0$, namely

$$\mathcal{T}_{\widehat{\sigma}} : L(\mathfrak{h}_1 \otimes \mathfrak{h}_2) \to L(\mathfrak{h}_1 \otimes \mathfrak{h}_2) \text{ is defined via } \mathcal{T}_{\widehat{\sigma}}(A \otimes B) := A \otimes B^{\top_{\widehat{\sigma}}} \tag{2.15}$$

and by linearity on the whole space $L(\mathfrak{h}_1 \otimes \mathfrak{h}_2)$. To define the $\widehat{\sigma}$-transpose $B^{\top_{\widehat{\sigma}}}$ we write $\widehat{\sigma} = \sum_{j=1}^J \sigma_j e_j \otimes \overline{e}_j$, where $\{ e_j \in \mathfrak{h}_2 \mid j = 1, .., J \}$ is an orthonormal basis in $\mathfrak{h}_2$, set $P_{jk} = e_j \otimes \overline{e}_k$, and set $P_{jk}^{\top_{\widehat{\sigma}}} = P_{kj}$, which defines $B^{\top_{\widehat{\sigma}}}$ by linearity. Clearly, $\mathcal{T}_{\widehat{\sigma}}\big(\mathcal{T}_{\widehat{\sigma}} \mathbb{Q}\big) = \mathbb{Q}$ and $\mathcal{T}_{\widehat{\sigma}} \mathbb{Q}$ is Hermitian if and only if $\mathbb{Q}$ is Hermitian.

Moreover, we define a $\widehat{\sigma}$-related operator $\mathcal{Y}_{\widehat{\sigma}}$ from $L(\mathfrak{h}_1 \otimes \mathfrak{h}_2)$ into itself via

$$\mathcal{Y}_{\widehat{\sigma}} \mathbb{Q} := (\mathbf{1}_{\mathfrak{h}_1} \otimes \widehat{\sigma}^{1/2}) \big(\mathcal{T}_{\widehat{\sigma}} \mathbb{Q}\big) (\mathbf{1}_{\mathfrak{h}_1} \otimes \widehat{\sigma}^{1/2}), \tag{2.16}$$

With $P_{jk} = e_j \otimes \overline{e}_k$ from above, every $\mathbb{Q} \in L(\mathfrak{h}_1 \otimes \mathfrak{h}_2)$ has the unique representation $\mathbb{Q} = \sum_{j,k=1}^J Q_{jk} \otimes P_{jk}$, and we obtain the formulas

$$\mathcal{T}_{\widehat{\sigma}} \mathbb{Q} = \sum_{j,k=1}^J Q_{kj} \otimes P_{jk} \text{ and } \mathcal{Y}_{\widehat{\sigma}} \mathbb{Q} = \sum_{j,k=1}^J \widetilde{Q}_{jk} \otimes P_{jk} \text{ with } \widetilde{Q}_{jk} = (\sigma_j \sigma_k)^{1/2} Q_{kj}. \tag{2.17}$$

The following result indicates how the partial $\widehat{\sigma}$-transpose interacts with the commutator of two Hermitian operators. It shows that a representation (2.10) for $\mathcal{L}$ in terms of $\mathbb{Q}$ and $\widehat{\sigma}$ is equivalent to a representation in terms of $\mathcal{Y}_{\widehat{\sigma}} \mathbb{Q}$ and $\widehat{\sigma}^{-1}$.

Lemma 2.6 *Consider $\widehat{\sigma} \in \mathrm{Herm}(\mathfrak{h}_2)$ with $\widehat{\sigma} > 0$. For $\mathbb{Q} \in L(\mathfrak{h}_1 \otimes \mathfrak{h}_2)$ we have*

$$\mathcal{T}_{\widehat{\sigma}}\big([\mathbb{Q}, A \otimes \widehat{\sigma}]\big) = \big(\mathbf{1}_{\mathfrak{h}_1} \otimes \widehat{\sigma}^{1/2}\big) [\mathcal{Y}_{\widehat{\sigma}} \mathbb{Q}, A \otimes \widehat{\sigma}^{-1}] \big(\mathbf{1}_{\mathfrak{h}_1} \otimes \widehat{\sigma}^{1/2}\big) \text{ for all } A \in L(\mathfrak{h}_1). \tag{2.18}$$

In particular, we have an equivalence between the commutation relations

$$[\mathbb{Q}, \widehat{\rho}_\beta \otimes \widehat{\sigma}] = 0 \quad \Longleftrightarrow \quad [\mathcal{Y}_{\widehat{\sigma}} \mathbb{Q}, \widehat{\rho}_\beta \otimes \widehat{\sigma}^{-1}] = 0 \tag{2.19}$$

and the dual representations of the compact representation of Lindblad operators:

$$\mathrm{Tr}_{\mathfrak{h}_2} \big[\mathbb{Q}, [\mathbb{Q}, A \otimes \sigma]\big] \;=\; \mathrm{Tr}_{\mathfrak{h}_2} \big[\mathcal{Y}_{\widehat{\sigma}} \mathbb{Q}, [\mathcal{Y}_{\widehat{\sigma}} \mathbb{Q}, A \otimes \widehat{\sigma}^{-1}]\big]. \tag{2.20}$$

Proof: To simplify the notation we abbreviate $M_{\widehat{\sigma}} := \mathbf{1}_{\mathfrak{h}_1} \otimes \sigma^{1/2}$.

For establishing (2.18), we can use linearity such that it is sufficient to consider the case $\mathbb{Q} = Q_{kl} \otimes P_{kl}$, which gives

$$\mathcal{T}_{\widehat{\sigma}} \big[\mathbb{Q}, A \otimes \widehat{\sigma}\big] = \sigma_l (Q_{kl} A) \otimes P_{lk} - \sigma_k (A Q_{kl}) \otimes P_{lk}.$$

Moreover, using $\mathcal{Y}_{\widehat\sigma}\mathbb{Q} = (\sigma_k\sigma_l)^{1/2}Q_{kl}\otimes P_{lk}$, we find

$$\big[\mathcal{Y}_{\widehat\sigma}\mathbb{Q}, A\otimes\widehat\sigma^{-1}\big] = (\sigma_l/\sigma_k)^{1/2}(Q_{kl}A)\otimes P_{lk} - (\sigma_k/\sigma_l)^{1/2}(AQ_{kl})\otimes P_{lk}.$$

Since multiplying this expression from the left and from the right by $M_{\widehat\sigma}$ reduces to multiplying by $(\sigma_k\sigma_l)^{1/2}$, we see that identity (2.18) is established.

Clearly, (2.19) follows from (2.18) by choosing $A = \widehat\rho_\beta$ and using that $M_{\widehat\sigma}$ is invertible.

Identity (2.20) follows by recalling the relation (2.12), which gives

$$-\operatorname{Tr}_{\mathfrak{h}_2}\big[\mathbb{Q}, [\mathbb{Q}, A\otimes\sigma]\big] = \sum\nolimits_{k,l=1}^{J}\sigma_l\big([Q_{kl}A, Q_{kl}^*] + [Q_{kl}, AQ_{kl}^*]\big).$$

Applying the same formula but with $\mathbb{Q}$ and $\widehat\sigma$ replaced by $\mathcal{Y}_{\widehat\sigma}\mathbb{Q}$ and $\widehat\sigma^{-1}$ we simply have to replace Q_{kl} by $\widetilde{Q}_{kl} = (\sigma_k\sigma_l)^{1/2}Q_{lk}$ and the eigenvalues σ_l by $1/\sigma_l$. We then find the same result, and (2.20) is proved. ∎

We now come to our representation of DBC Lindbladians with the choice $\widehat\sigma = \widehat\rho_\beta$ or $\widehat\sigma = \widehat{\rho_\beta}^{-1}$, which are both useful and have a natural interpretation. In the first case, we can use the fact that for all $\rho \in \mathfrak{R} \subset L(\mathfrak{h})$ the tensor product $\rho\otimes\widehat\rho_\beta$ is again a density matrix, but now on the Hilbert space $\mathfrak{h}\otimes\mathfrak{h}$. In the second case the matrix $\rho\otimes\widehat{\rho_\beta}^{-1}$ can be seen as a non-commutative counterpart of the relative density $\varrho(x) = u(x)/U^{\mathrm{eq}}(x)$ in the Fokker-Planck equation or of the relative density $(p_n/w_n^{\mathrm{eq}})_{n=1,..,N}$ for discrete Markov processes, see Section 3.1. Note also that the two commutator relations

$$[\mathbb{Q}, \widehat\rho_\beta\otimes\widehat\rho_\beta] = 0 \quad\text{and}\quad [\widetilde{\mathbb{Q}}, \widehat\rho_\beta\otimes\widehat{\rho_\beta}^{-1}] = 0$$

look quite different, since $\widehat\rho_\beta\otimes\widehat\rho_\beta$ has the eigenvalues $\frac{1}{Z_\beta}\mathrm{e}^{-\beta(\varepsilon_j+\varepsilon_k)}$ while $\widehat\rho_\beta\otimes\widehat{\rho_\beta}^{-1}$ has the eigenvalues $\frac{1}{Z_\beta}\mathrm{e}^{-\beta(\varepsilon_j-\varepsilon_k)}$. So the latter appears closer to the relevant eigenpairs $(\omega, Q) \in \mathfrak{E}(H)$. However, we will see in the following theorem that there is a one-to-one correspondence between all possible $\mathbb{Q}$ and $\widetilde{\mathbb{Q}}$. Its proof is based on the previous lemma.

Theorem 2.7 (Compact representation of $\mathcal{L}$ with DBC) *Let $\mathcal{L}$ be a DBC Lindblad operator with respect to $\widehat\rho_\beta \in L(\mathfrak{h})$. Then, there exists $\mathbb{Q} \in \mathrm{Herm}(\mathfrak{h}\otimes\mathfrak{h}_2)$ with $\mathfrak{h}_2 = \mathfrak{h}$ satisfying the commutator relation $[\mathbb{Q}, \widehat\rho_\beta\otimes\widehat\rho_\beta] = 0$ such that the representation*

$$\mathcal{L}\rho = -\operatorname{Tr}_{\mathfrak{h}_2}\Big(\big[\mathbb{Q}, [\mathbb{Q}, \rho\otimes\widehat\rho_\beta]\big]\Big)$$

holds. Moreover, choosing $\widetilde{\mathbb{Q}} = \mathcal{Y}_{\widehat\rho_\beta}\mathbb{Q}$ as in Lemma 2.6, we have the alternative representation

$$\mathcal{L}\rho = -\operatorname{Tr}_{\mathfrak{h}_2}\Big(\big[\widetilde{\mathbb{Q}}, [\widetilde{\mathbb{Q}}, \rho\otimes\widehat{\rho_\beta}^{-1}]\big]\Big).$$

Proof: By [KF*77] every DBC Lindblad operator can be written in the form

$$\mathcal{L}(\rho) = \sum_{ij,mn} M_{ij,mn}([P_{ij}\rho, P_{mn}^*] + [P_{ij}, \rho P_{mn}^*])$$

with $P_{ij} = h_i\otimes\overline{h}_j$, where h_i are the eigenvectors of $\widehat\rho_\beta$, and $M_{ij,mn}$ satisfy

(i) $\overline{M}_{mn,ij} = M_{ij,mn}$, (ii) $\varepsilon_j - \varepsilon_i \neq \varepsilon_n - \varepsilon_m \implies M_{ij,mn} = 0$,
(iii) $M_{nm,ji} = \mathrm{e}^{-\beta\omega}M_{ij,mn}$ with $\omega = \varepsilon_j - \varepsilon_i = \varepsilon_n - \varepsilon_m$.

We construct the Hermitian operator $\mathbb{Q}$ in the form $\mathbb{Q} = \sum_{i,j,m,n} A_{ij,kl} P_{ij} \otimes P^*_{kl}$. Hence,

$$
\begin{aligned}
[\mathbb{Q}, \widehat{\rho}_\beta \otimes \widehat{\rho}_\beta] = 0 \quad &\Longleftrightarrow \quad \Big(A_{ij,kl} = 0 \text{ whenever } \varepsilon_j - \varepsilon_i \neq \varepsilon_l - \varepsilon_k \Big), \\
\mathbb{Q}^* = \mathbb{Q} \quad &\Longleftrightarrow \quad \overline{A}_{ij,kl} = A_{ji,lk}.
\end{aligned}
$$

To this end we define

$$
\widetilde{M}_{ij,mn} = Z_\beta^2 \, \mathrm{e}^{\beta(\varepsilon_i + \varepsilon_m)/2} M_{ij,mn}.
$$

Then $\widetilde{M}_{ij,mn} = \widetilde{M}_{nm,ji} = \overline{\widetilde{M}}_{ji,mn}$. This symmetry property remains true for all powers of $\widetilde{M}$ and thus for $\widetilde{M}^{\frac{1}{2}}$ as well. Define $A_{ij,kl} = \mathrm{e}^{\beta \frac{\varepsilon_k - \varepsilon_i}{2}} (\widetilde{M}^{\frac{1}{2}})_{ij,kl}$. Then,

$$
\begin{aligned}
A_{ji,lk} &= \mathrm{e}^{\beta \frac{\varepsilon_l - \varepsilon_j}{2}} (\widetilde{M}^{\frac{1}{2}})_{ji,lk} = \mathrm{e}^{\beta \frac{\varepsilon_l - \varepsilon_j}{2}} \overline{(\widetilde{M}^{\frac{1}{2}})_{ij,kl}} \\
&= \mathrm{e}^{\beta \frac{\varepsilon_l - \varepsilon_k}{2} - \beta \frac{\varepsilon_j - \varepsilon_i}{2}} \overline{A_{ij,kl}} = \mathrm{e}^{\beta \frac{\omega - \omega}{2}} \overline{A_{ij,kl}}
\end{aligned}
$$

Thus the corresponding $\mathbb{Q}$ is Hermitian and $A_{ij,kl} = 0 \;$ if $\varepsilon_j - \varepsilon_i \neq \varepsilon_l - \varepsilon_k$ follows from condition (2) on $M_{ij,mn}$. Finally

$$
\begin{aligned}
\frac{1}{Z_\beta^2} \sum_{k,l} A_{ij,kl} \overline{A_{mn,kl}} \mathrm{e}^{-\beta \varepsilon_k} &= \frac{1}{Z_\beta^2} \sum_{k,l} \mathrm{e}^{\beta \frac{\varepsilon_k - \varepsilon_i}{2}} (\widetilde{M}^{\frac{1}{2}})_{ij,kl} \cdot \mathrm{e}^{\beta \frac{\varepsilon_k - \varepsilon_m}{2}} \overline{(\widetilde{M}^{\frac{1}{2}})_{mn,kl}} \mathrm{e}^{-\beta \varepsilon_k} \\
= \mathrm{e}^{-\beta \frac{\varepsilon_i + \varepsilon_m}{2}} \frac{1}{Z_\beta^2} \sum_{k,l} (\widetilde{M}^{\frac{1}{2}})_{ij,kl} (\widetilde{M}^{\frac{1}{2}})_{kl,mn} &= \mathrm{e}^{-\beta \frac{\varepsilon_i + \varepsilon_m}{2}} \frac{1}{Z_\beta^2} \widetilde{M}_{ij,mn} = H_{ij,mn}
\end{aligned}
$$

which means that

$$
\mathcal{L}\rho = \sum_{ij,mn} M_{ij,mn} \big([P_{ij}\rho, P^*_{mn}] + [P_{ij}, \rho P^*_{mn}] \big) = - \operatorname{Tr}_{\mathfrak{h}_2} \Big(\big[\mathbb{Q}, [\mathbb{Q}, \rho \otimes \widehat{\rho}_\beta] \big] \Big).
$$

This establishes the first representation based on $\mathbb{Q}$ and $\widehat{\rho}_\beta$. The second representation involving $\widetilde{\mathbb{Q}}_{\widehat{\rho}_\beta}$ and $\widehat{\rho}_\beta^{-1}$ follows simply by applying (2.20) to the case $\sigma = \widehat{\rho}_\beta$. ■

2.4 Examples of Lindblad operators and equations

Here we give two elementary examples to highlight the structures and to come back to them in later sections. We refer to [BNT08, BaN08, BaN12, AlJ14] for general discussions of the dynamics of Lindblad equations with or without DBC. Even without explicitly mentioning the DBC, it was already observed in [Dav74, Thm. 4.4] that under the additional assumption that the eigenvalues of H are all simple, the diagonal elements $\rho_{jj}(t)$, $j = 1, ..., N$, of $\rho(t)$ with respect to the eigenbasis of H evolve according to a classical Markov process, see also [Ali76, Eqn. (21)].

2.4.1 The Bloch sphere for the case $N = 2$

For the case $\mathfrak{h} = \mathbb{C}^2$ and $H = \operatorname{diag}(\varepsilon_1, \varepsilon_2)$ with $\varepsilon_1 \neq \varepsilon_2$ we characterize all DBC Lindbladians $\mathcal{L}$ with respect to $\widehat{\rho}_\beta$. For this we use the Pauli matrices

$$
\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
$$

and the operators $\sigma_\pm = \frac{1}{2}(\sigma_1 \pm \sigma_2)$. Then, all $\mathcal{L}$ satisfying the DBC have the form

$$\begin{aligned}\mathcal{L}_d(\rho) = \frac{\gamma}{2}\Big(\mathrm{e}^{-\beta\varepsilon_1}\big([\sigma_+\rho,\sigma_-]+[\sigma_+,\rho\sigma_-]\big)+\mathrm{e}^{-\beta\varepsilon_2}\big([\sigma_-\rho,\sigma_+]+[\sigma_-,\rho\sigma_+]\big)\Big)\\ +\frac{\delta}{2}\big([\sigma_3\rho,\sigma_3]+[\sigma_3,\rho\sigma_3]\big),\end{aligned} \tag{2.21}$$

which are simply two building blocks with $Q=\sigma_+$, $Q^*=\sigma_-$, and $W=\sigma_3$.

It is more convenient to write the above generator in terms of real-valued Bloch coordinates $\mathbf{a}\in\mathbb{R}^3$ via $\rho(\mathbf{a})=\frac{1}{2}\mathrm{id}+\frac{1}{2}\sum_{i=1}^3 a_i\cdot\sigma_i$. The positivity $\rho\geq 0$ is equivalent to $|\mathbf{a}|\leq 1$. The Lindblad equation $\dot\rho=\mathcal{L}_d(\rho)$ reads $\dot{\mathbf{a}}=R\mathbf{a}+\mathbf{k}$ in Bloch coordinates with

$$R=\begin{pmatrix}-(\gamma{+}2\delta) & 0 & 0\\ 0 & -(\gamma{+}2\delta) & 0\\ 0 & 0 & -2\gamma\end{pmatrix},\quad \mathbf{k}=\begin{pmatrix}0\\0\\2\gamma\overline{w}\end{pmatrix} \tag{2.22}$$

and with $\overline{w_\beta}=\mathrm{e}^{-\beta\varepsilon_1}-\mathrm{e}^{-\beta\varepsilon_2}$. This is the dissipative part of the well-known phenomenological Bloch equations. The longitudinal and transverse relaxation times T_1 and T_2 are given by $T_1=\frac{1}{2\gamma}$ and $T_2=\frac{1}{\gamma+2\delta}$. They satisfy the inequality $T_1\geq\frac{1}{2}T_2$.

2.4.2 A nontrivial case

In this example we give a case where an eigenvalue $\omega\neq 0$ of $A\mapsto[A,H]$ is not simple, which allows for a nontrivial coupling between four energy levels.

In $\mathfrak{h}=\mathbb{C}^4$ we choose $H=\sum_{i=1}^4\varepsilon_i h_i$ with $\varepsilon_4=10$, $\varepsilon_3=9$, $\varepsilon_2=2$, $\varepsilon_1=1$, and $Q=h_1\otimes\overline{h}_2+h_3\otimes\overline{h}_4$. Using $\varepsilon_4{-}\varepsilon_3=\varepsilon_2{-}\varepsilon_1=1$ we have $(1,Q)\in\mathfrak{E}(H)$. Then, by Proposition 2.2(b) we see that

$$\dot\rho=\mathcal{M}_Q^\beta\rho=\mathrm{e}^{\frac{\beta}{2}}([QA,Q^*]+[Q,AQ^*])+\mathrm{e}^{-\frac{\beta}{2}}([Q^*A,Q]+[Q^*,AQ]) \tag{2.23}$$

satisfies the DBC with respect to $\widehat{\rho}_\beta$. Let us rewrite the above equation in coordinates. The diagonal elements form a Markov chain

$$\begin{aligned}\dot\rho_{11}&=-\mathrm{e}^{-\frac{\beta}{2}}\rho_{11}+\mathrm{e}^{\frac{\beta}{2}}\rho_{22} & \qquad \dot\rho_{33}&=-\mathrm{e}^{-\frac{\beta}{2}}\rho_{33}+\mathrm{e}^{\frac{\beta}{2}}\rho_{44}\\ \dot\rho_{22}&=+\mathrm{e}^{-\frac{\beta}{2}}\rho_{11}-\mathrm{e}^{\frac{\beta}{2}}\rho_{22} & \dot\rho_{44}&=+\mathrm{e}^{-\frac{\beta}{2}}\rho_{33}-\mathrm{e}^{\frac{\beta}{2}}\rho_{44}\end{aligned}$$

and the evolution of the off-diagonal elements is given by

$$\dot\rho_{13}=-\mathrm{e}^{-\frac{\beta}{2}}\rho_{13}+\mathrm{e}^{\frac{\beta}{2}}\rho_{24}\quad \dot\rho_{24}=+\mathrm{e}^{-\frac{\beta}{2}}\rho_{13}-\mathrm{e}^{\frac{\beta}{2}}\rho_{24}$$

and $\dot\rho_{kl}=-\cosh\frac{\beta}{2}\,\rho_{kl}$ for $(k,l)\notin\{(1,3),(3,1),(2,4),(4,2)\}$. This example shows, that non-diagonal elements (here ρ_{13} and ρ_{24}) can couple, if the energy differences are the same. Note that ρ_{11} and ρ_{22} are decoupled from ρ_{33} and ρ_{44}. Thus $\widehat{\rho}_\beta$ is not the only equilibrium of (2.23). This is also the reason why ρ_{13} and ρ_{24} do not decay to 0, contrary to the other off-diagonal elements.

In the presence of symmetries or conserved quantities even more complicated situations are possible, see [AlJ14].

3 An entropic gradient structure for the Lindblad equation

3.1 Entropic gradient structures for classical Markov processes

The entropic gradient structure for master equations for classical Markov processes goes back to the seminal work [JKO97, JKO98], where the Fokker-Planck equation

$$\dot u = \mathrm{div}\Big(a(x)\big(\nabla u + u\nabla V(x)\big)\Big)$$

for the probability density $u(t,x)\geq 0$ was written as a gradient system with respect to the Wasserstein distance. Here $a(x)\in\mathbb{R}^{d\times d}$ is a symmetric and positive definite diffusion matrix. The gradient structure has the form

$$\dot u = -\mathbb{K}_\mathrm{W}(u)\,\mathrm{D}\mathcal{F}(u),$$

where $\mathcal{F}$ is the free energy (or relative entropy with respect to the equilibrium density $U^\mathrm{eq}(x) = \mathrm{e}^{-V(x)}$) and $\mathbb{K}_\mathrm{W}$ is the Onsager operator associated with the Wasserstein distance, namely

$$\begin{aligned}&\mathcal{F}(u) = \int_{\mathbb{R}^d}\Big(u(x)\log u(x) + V(x)u(x)\Big)\,\mathrm{d}x = \int_{\mathbb{R}^d} u(x)\log\big(u(x)/U^\mathrm{eq}(x)\big)\,\mathrm{d}x,\\ &\mathbb{K}_\mathrm{W}(u)\xi = -\,\mathrm{div}\,\big(u\,a(x)\,\nabla\xi\big).\end{aligned}$$

A related gradient structure for time-continuous Markov processes on a discrete state space $\{1,\dots,N\}$ was found independently by the three groups [Maa11, ErM12], [CH*12], and [Mie11b, Mie13b]. In this case the Kolmogorov forward equation for the probability vector $p(t)\in\{\,(p_1,\dots,p_N)\in[0,1]^N\,|\,\sum_{n=1}^N p_n = 1\,\}$ is the linear system

$$\dot p = Lp, \quad \text{where } L_{nm}\geq 0 \text{ for } n\neq m \text{ and } L^\top(1,1,..,1)^\top = 0.$$

The detailed balance condition for L and the equilibrium w^eq reads

$$Lw^\mathrm{eq} = 0 \text{ with } w_n^\mathrm{eq}>0 \quad\text{and}\quad \kappa_{nm} := L_{nm}w_m^\mathrm{eq} = L_{mn}w_n^\mathrm{eq} \text{ for all } n,m\in\{1,..,N\}.$$

The entropic gradient structure is defined in terms of the relative entropy $\mathcal{E}(p)=\mathcal{H}(p|w^\mathrm{eq})$ and the Onsager operator $\mathbb{K}_\mathrm{M}(p)$ with

$$\mathcal{E}(p) = \sum_{n=1}^N p_n\log\big(p_n/w_n^\mathrm{eq}\big) \text{ and } \mathbb{K}_\mathrm{M}(p) = \sum_{m>n}\kappa_{nm}\Lambda\big(\tfrac{p_n}{w_n^\mathrm{eq}},\tfrac{p_m}{w_m^\mathrm{eq}}\big)\Big(e_n{-}e_m\Big)\otimes\Big(e_n{-}e_m\Big),$$

where $\Lambda(a,b)\geq 0$ denotes the ***logarithmic mean of*** a ***and*** b:

$$\Lambda(a,b) = \int_0^1 a^s\,b^{1-s}\,\mathrm{d}s = \frac{a\;-\;b}{\log a - \log b}. \tag{3.1}$$

Note that using $\mathrm{D}\mathcal{E}(p) = \big(\log p_n - \log w_n^\mathrm{eq}\big)_{n=1,..,N}$, the relation $\Lambda(a,b)\big(\log a - \log b\big) = a-b$, and the detailed balance condition easily yield the identity $Lp = -\mathbb{K}_\mathrm{M}(p)\mathrm{D}\mathcal{E}(p)$.

3.2 The Kubo-Mori operator $\mathcal{C}_\rho$ and the generalization $\mathcal{D}_\rho^\alpha$

The development of an analogous gradient structure for the dissipative part of the Lindblad equation was less successful. The attempts in [Ött10, Ött11, Mie13a, Mie15] produced nonlinear terms, unless the Hamiltonian H is a multiple of $\mathbf{1}_{\mathfrak{h}}$ (as in [CaM14] or more generally only the building blocks $\mathcal{S}_W$ in Proposition 2.2 are used). All of these works involve the Kubo-Mori operator $\mathcal{C}_\rho : L(\mathfrak{h}) \to L(\mathfrak{h})$ as a generalization of the multiplication with u in the Fokker-Planck equation and the logarithmic mean $\Lambda(\frac{p_n}{w_n^{\mathrm{eq}}}, \frac{p_m}{w_m^{\mathrm{eq}}})$. It is defined via

$$\mathcal{C}_\rho A := \int_0^1 \rho^s \, A \, \rho^{1-s} \, \mathrm{d}s \;=\; \sum_{n,m=1}^{N} \Lambda(r_n, r_m) \left\langle \psi_n | A \psi_m \right\rangle |\psi_n\rangle \left\langle \psi \right|_m,$$

if ρ is given by (2.1).

One major property of $\mathcal{C}_\rho$ is that it satisfies the analog of the identities

$$u \nabla \log \left(u/\mathrm{e}^{-V} \right) = \nabla u + u \nabla V \quad \text{and} \quad \Lambda(a,b)(\log a - \log b) = a - b \tag{3.2}$$

for the classical Markov setting. Note that the right-hand sides are linear in u and (a,b), respectively. For all $Q \in L(\mathfrak{h})$ the operator $\mathcal{C}_\rho$ satisfies a similar "miracle identity", namely

$$\mathcal{C}_\rho [Q, \log \rho] = [Q, \rho], \tag{3.3}$$

see [Ött10, Ött11, Mie13a, Mie15]. We will provide a proof of a more general version of this identity in Proposition 3.1.

This relation works well (see [CaM14]) if we are using the total entropy $\mathcal{S}_0(\rho) = -\operatorname{Tr}(\rho \log \rho)$ which has the derivative $\mathrm{D}\mathcal{S}(\rho) = -\log \rho$ (up to an identity which is irrelevant since $\operatorname{Tr} \rho = 1$). However, for relative entropies of the form $\mathcal{S}_\beta(\rho) = -\operatorname{Tr}(\beta H \rho + \rho \log \rho)$ we have

$$\mathrm{D}\mathcal{S}_\beta(\rho) = -\beta H - \log \rho \quad \rightsquigarrow \quad \mathcal{C}_\rho \left[Q, \mathrm{D}\mathcal{S}_\beta(\rho) \right] = -[Q, \rho] - \mathcal{C}_\rho [Q, H].$$

Thus, the right-hand side is no longer linear, unless Q commutes with H. The Fokker–Planck equation studied in [CaM14] has $H = 0$ and hence falls into this class, i.e. the Fokker-Planck equation is indeed a linear Lindblad equation. However, the models studied in [Ött10, Ött11, Mie13a, Mie15] include the nonsmooth term $\mathcal{C}_\rho[Q, H]$, which is continuous but not Hölder continuous, so the existence theory developed in [Mie13a, Sec. 21.6] is nontrivial and uniqueness of solutions couldn't be established.

We now show that it is possible to use variants of $\mathcal{C}_\rho$ such that for $(\omega, Q) \in \mathfrak{E}(H)$ we obtain a suitable counterpart of (3.2). Indeed we will be able to show that all DBC Lindbladians can be written in terms of these variants of $\mathcal{C}_\rho$. The variant of $\mathcal{C}_\rho$ we are using is defined in terms of the tilted operator $\mathcal{D}_\rho^\alpha$, where $\alpha \in \mathbb{R}$ will be related to an energy difference:

$$\mathcal{D}_\rho^\alpha A := \mathrm{e}^{-\alpha/2} \int_0^1 \mathrm{e}^{s\alpha} \rho^s A \, \rho^{1-s} \, \mathrm{d}s \;=\; \sum_{n,k=1}^{N} \Lambda\big(\mathrm{e}^{\alpha/2} r_n \, , \, \mathrm{e}^{-\alpha/2} r_k \big) \left\langle \psi_n | A | \psi_k \right\rangle \psi_n \otimes \overline{\psi}_k, \tag{3.4}$$

if ρ is given by (2.1). Again the logarithmic mean $\Lambda(a,b)$ from (3.1) is involved, but now weighted with $\mathrm{e}^{\pm\alpha/2}$.

The generalized miracle identity is given in the following result (3.7), which again shows that applying $\mathcal{D}_\rho^\alpha$ to a commutator with $\log \rho$ plus a suitable correction provides a linear expression, i.e. the nonlinearities involved in $\log \rho$ and $\mathcal{D}_\rho^\alpha$ cancel each other.

Proposition 3.1 *For all $\alpha \in \mathbb{R}$, $A, Q \in L(\mathfrak{h})$, and $\rho \in \mathfrak{R}_N$ we have the identities*

$$\big(\mathcal{D}_\rho^\alpha\big)^* = \mathcal{D}_\rho^\alpha \quad \text{and} \quad \big(\mathcal{D}_\rho^\alpha A^*\big)^* = \mathcal{D}_\rho^{-\alpha} A, \tag{3.5}$$

$$\langle\!\langle\, A \,\|\, \mathcal{D}_\rho^\alpha A \,\rangle\!\rangle \geq 0, \tag{3.6}$$

$$\mathcal{D}_\rho^\alpha\big([Q, \log \rho] - \alpha Q\big) = \mathrm{e}^{-\alpha/2} Q\rho - \mathrm{e}^{\alpha/2}\rho Q. \tag{3.7}$$

From the proof it is clear, that the generalized miracle identity (3.7) also holds for $\alpha \in \mathbb{C}$, but our use will be restricted to real-valued energy levels.

Proof: The relations in (3.5) follow directly from the definition. For (3.6) we use

$$\begin{aligned}\langle\!\langle\, A \,\|\, \mathcal{D}_\rho^\alpha A \,\rangle\!\rangle &= \mathrm{e}^{-\alpha/2} \int_0^1 \mathrm{e}^{s\alpha} \langle\!\langle\, A \,\|\, \rho^s A \rho^{1-s} \,\rangle\!\rangle \,\mathrm{d}s \\ &= \int_0^1 \mathrm{e}^{\alpha(s-1/2)}\, \mathrm{Tr}\,\big((\rho^{s/2} A \rho^{s/2})^* \rho^{s/2} A \rho^{s/2} \rho^{1-2s}\big) \,\mathrm{d}s \geq 0,\end{aligned}$$

since the integrand is non-negative for all $s \in [0,1]$.

For (3.7), we generalize the simple proof of (3.3) from [Mie13a, Prop. 21.1], write $\Lambda = \log \rho$, and use the fact that the integrand defining $\mathcal{D}_\rho^\alpha$ can be written as a total derivative with respect to $s \in [0,1]$:

$$\begin{aligned}&\mathcal{D}_\rho^\alpha\big([Q, \log \rho] - \alpha Q\big) = \mathrm{e}^{-\alpha/2} \int_0^1 \mathrm{e}^{\alpha s} \mathrm{e}^{s\Lambda}\big(Q\Lambda - \Lambda Q - \alpha \Lambda\big) \mathrm{e}^{(1-s)\Lambda} \,\mathrm{d}s \\ &= -\mathrm{e}^{-\alpha/2} \int_0^1 \Big(\mathrm{e}^{\alpha s} \mathrm{e}^{s\Lambda} (\Lambda{+}\alpha I) Q \mathrm{e}^{(1-s)\Lambda} + \mathrm{e}^{\alpha s} \mathrm{e}^{s\Lambda} Q \big(-\Lambda\big) \mathrm{e}^{(1-s)\Lambda}\Big) \,\mathrm{d}s \\ &= -\mathrm{e}^{-\alpha/2} \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}\Big(\mathrm{e}^{(\Lambda+\alpha I)s} Q \mathrm{e}^{(1-s)\Lambda}\Big) \,\mathrm{d}s \;=\; \mathrm{e}^{-\alpha/2}\big(Q\mathrm{e}^{\Lambda} - \mathrm{e}^{\Lambda+\alpha I} Q\big) \\ &= \mathrm{e}^{-\alpha/2} Q\rho - \mathrm{e}^{\alpha/2}\rho Q.\end{aligned}$$

This is the desired result. ■

The following result follows immediately from the above proposition by setting $\alpha = -\beta\omega$. It will be the basis for our construction of the entropic gradient structure.

Corollary 3.2 *Assume $\beta > 0$ and that $(\omega, H) \in \mathfrak{E}(H)$, that is $[Q, H] = \omega Q$, then*

$$\mathcal{D}_\rho^{-\beta\omega}\,\big[\, Q \,,\, \log \rho + \beta H \,\big] \;=\; \mathrm{e}^{\beta\omega/2} Q\rho - \mathrm{e}^{-\beta\omega/2}\rho Q. \tag{3.8}$$

The next lemma shows that $\mathcal{D}_\rho^\alpha$ appears naturally if we tensorize ρ with a diagonal matrix, and thus connects our construction with that in Section 2.3.

Lemma 3.3 *For all $\rho \in \mathfrak{R}$ and all $\alpha \in \mathbb{R}$ we have*

$$\mathcal{C}_{\begin{pmatrix} \mathrm{e}^{\alpha/2}\rho & 0 \\ 0 & \mathrm{e}^{-\alpha/2}\rho \end{pmatrix}} \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{\alpha/2}\mathcal{C}_\rho A & \mathcal{D}_\rho^\alpha B \\ \mathcal{D}_\rho^{-\alpha} C & \mathrm{e}^{-\alpha/2}\mathcal{C}_\rho D \end{pmatrix}.$$

Proof: This follows simply by using the identity (for $a, b > 0$)

$$\begin{pmatrix} a\rho & 0 \\ 0 & b\rho \end{pmatrix}^s = \begin{pmatrix} a^s\rho^s & 0 \\ 0 & b^s\rho^s \end{pmatrix}$$

and the definitions of $\mathcal{C}_{\left(\begin{smallmatrix} \rho_1 & 0 \\ 0 & \rho_2 \end{smallmatrix}\right)}$ and $\mathcal{D}^\alpha_\rho$ from above. ∎

As was pointed out in Section 2.3 every Lindblad operator can be written as the sum of partial traces of double commutators on a larger tensor product space. This enlarged space has the advantage, that the miracle identity (3.7) becomes very elegant and more transparent, when taking the original miracle identity for granted.

Theorem 3.4 (Generalized miracle identity) *Consider* $\mathbb{Q} \in \mathrm{Herm}(\mathfrak{h}_1 \otimes \mathfrak{h}_2)$, $\widehat{\rho} \in \mathrm{Herm}(\mathfrak{h}_1)$ *and* $\widehat{\sigma} \in \mathrm{Herm}(\mathfrak{h}_2)$ *with* $\widehat{\rho}, \widehat{\sigma} > 0$ *satisfying the commutator relation* (2.11)*, i.e.* $[\mathbb{Q}, \widehat{\rho}_\beta \otimes \widehat{\sigma}] = 0$*. Then, for all* $\rho \in \mathfrak{R}$ *we have the identity*

$$\mathcal{C}_{\rho\otimes\widehat{\sigma}}\big[\mathbb{Q}, (\log\rho - \log\widehat{\rho}_\beta)\otimes \mathbf{1}_{\mathfrak{h}_2}\big] = [\mathbb{Q}, \rho\otimes\widehat{\sigma}]\,. \tag{3.9}$$

Proof: Using Lemma 2.4 in "$\overset{\star}{=}$" below we obtain the following chain of identities:

$$\begin{aligned}
&\mathcal{C}_{\rho\otimes\widehat{\sigma}}[\mathbb{Q}, (\log\rho - \log\widehat{\rho})\otimes\mathbf{1}_{\mathfrak{h}_2}] = \mathcal{C}_{\rho\otimes\widehat{\sigma}}[\mathbb{Q}, (\log\rho)\otimes\mathbf{1}_{\mathfrak{h}_2}] - \mathcal{C}_{\rho\otimes\widehat{\sigma}}[\mathbb{Q}, (\log\widehat{\rho})\otimes\mathbf{1}_{\mathfrak{h}_2}] \\
&\overset{\star}{=} \mathcal{C}_{\rho\otimes\widehat{\sigma}}\left[\mathbb{Q}, (\log\rho)\otimes\mathbf{1}_{\mathfrak{h}_2}\right] + \mathcal{C}_{\rho\otimes\widehat{\sigma}}[\mathbb{Q}, \mathbf{1}_{\mathfrak{h}_1}\otimes(\log\widehat{\sigma})\big] \\
&= \mathcal{C}_{\rho\otimes\widehat{\sigma}}\big[\mathbb{Q}, (\log\rho)\otimes\mathbf{1}_{\mathfrak{h}_2} + \mathbf{1}_{\mathfrak{h}_1}\otimes(\log\widehat{\sigma})\big] = \mathcal{C}_{\rho\otimes\widehat{\sigma}}\left[\mathbb{Q}, \log(\rho\otimes\widehat{\sigma})\right] \overset{\circ}{=} [\mathbb{Q}, \rho\otimes\widehat{\sigma}]\,,
\end{aligned}$$

where "$\overset{\circ}{=}$" uses the classical miracle identity (3.3). ∎

We note that relation (3.8) in Corollary 3.2 is a direct consequence of Theorem 3.4 by setting

$$\mathbb{Q} = \begin{pmatrix} 0 & Q^* \\ Q & 0 \end{pmatrix} \quad \widehat{\sigma} = \begin{pmatrix} \mathrm{e}^{\beta\omega/2} & 0 \\ 0 & \mathrm{e}^{-\beta\omega/2} \end{pmatrix}.$$

3.3 Dissipation potential and Onsager operator

We now complete the task of writing the dissipative part $\mathcal{L}$ of any DBC Lindblad operator with respect to $\widehat{\rho}_\beta$ as a gradient of the relative entropy, namely

$$\mathcal{F}(\rho) = \mathcal{H}(\rho|\widehat{\rho}_\beta) := \mathrm{Tr}\Big(\rho\big(\log\rho - \log\widehat{\rho}_\beta\big)\Big) = \mathrm{Tr}\left(\rho\log\rho + \rho\,\beta H\right) + \log Z_\beta.$$

The aim is to construct an Onsager operator $\mathbb{K}(\rho)$ such that

$$\mathcal{L}\rho = -\mathbb{K}(\rho)\mathrm{D}\mathcal{F}(\rho) = -\mathbb{K}(\rho)\big(\log\rho + \beta H\big).$$

The symmetric and positive definite Onsager operator $\mathbb{K}(\rho)$ is most easily defined in terms of a non-negative and quadratic dual dissipation potential

$$\mathcal{R}^*(\rho, \xi) = \frac{1}{2}\langle\!\langle\, \xi \,\|\, \mathbb{K}(\rho)\xi \,\rangle\!\rangle.$$

Such a structure is conveniently written down in the compact tensor product formulation for Lindblad operators $\mathcal{L}$ as developed in Section 2.3, namely

$$\mathcal{L}\rho = -\operatorname{Tr}_{\mathfrak{h}_2}\Big(\big[\mathbb{Q},[\mathbb{Q},\rho\otimes\widehat{\sigma}]\big]\Big). \tag{3.10}$$

As a corollary we will also obtain the corresponding gradient structures for the building blocks of Proposition 2.2, namely

$$\mathcal{L}\rho = \sum_{j=1}^{J}\mathcal{M}^{\beta}_{Q_j}\,\rho \quad \text{where } (\omega_j,Q_j)\in\mathfrak{E}(H).$$

Indeed, each building block can be expressed in tensor form with $\widehat{\sigma}_j = 1$ or $\widehat{\sigma}_n \in \mathbb{R}^{2\times 2}$. If we construct a suitable $\mathcal{K}_j(\rho)$ for each of the building blocks, we can use the additivity principle for Onsager operators, i.e. the sum $\mathbb{K}(\rho) := \sum_{j=1}^{J}\mathcal{K}_j(\rho)$ is the desired total Onsager operator.

The tensorial representation (3.10) for DBC Lindblad operators with respect to $\widehat{\rho}_\beta$ and the tensorial miracle identity (3.9) lead us to the following general result.

Proposition 3.5 (Onsager operators and dissipation potentials) *For given $\mathbb{Q}$, $\widehat{\rho}_\beta$, and $\widehat{\sigma}$ satisfying the commutation relation $[\mathbb{Q},\widehat{\rho}_\beta\otimes\widehat{\sigma}] = 0$, we define the Onsager operator $\mathbb{K}(\rho) : \operatorname{Herm}(\mathfrak{h}_1) \to \operatorname{Herm}(\mathfrak{h}_1)$ and the dual dissipation potential $\mathcal{R}^*(\rho,\cdot) : \operatorname{Herm}(\mathfrak{h}_1) \to \mathbb{R}$ via*

$$\mathbb{K}(\rho)\xi := \operatorname{Tr}_{\mathfrak{h}_2}\Big(\big[\mathbb{Q},\mathcal{C}_{\rho\otimes\widehat{\sigma}}[\mathbb{Q},\xi\otimes\mathbf{1}_{\mathfrak{h}_2}]\big]\Big)$$
$$\mathcal{R}^*(\rho,\xi) := \frac{1}{2}\Big\langle\big[\mathbb{Q},\xi\otimes\mathbf{1}_{\mathfrak{h}_2}\big],\mathcal{C}_{\rho\otimes\widehat{\sigma}}\big[\mathbb{Q},\xi\otimes\mathbf{1}_{\mathfrak{h}_2}\big]\Big\rangle.$$

Then,

$$\mathbb{K}(\rho)(\log\rho - \log\widehat{\rho}_\beta) = \operatorname{Tr}_{\mathfrak{h}_2}([\mathbb{Q},[\mathbb{Q},\rho\otimes\widehat{\sigma}]]) \tag{3.11}$$

as well as

$$\mathbb{K}(\rho) = \mathbb{K}(\rho)^* \geq 0, \quad \mathbb{K}(\rho)\xi = \mathrm{D}_\xi\mathcal{R}^*(\rho,\xi), \quad \langle\xi,\mathbb{K}(\rho)\xi\rangle = 2\mathcal{R}^*(\rho,\xi) \geq 0.$$

Proof: We first observe that relation (3.11) follows by employing Theorem 3.4. The positivity of $\mathcal{R}^*$ is a special case of Proposition 3.1 for $\alpha = 0$, i.e. $\mathcal{C}_{\rho\otimes\widehat{\sigma}} \geq 0$. Finally, we obtain $\mathbb{K}(\rho)\xi = \mathrm{D}_\xi\mathcal{R}^*(\rho,\xi)$ by noting that $\operatorname{Tr}_{\mathfrak{h}_2}$ is adjoint to $A \mapsto A\otimes\mathbf{1}_{\mathfrak{h}_2}$. This then shows $\mathbb{K} = \mathbb{K}^* \geq 0$. ■

Note that the operators $\mathbb{Q}$ and $\widehat{\sigma}$ strongly depend on H and β since they have to satisfy the commutation relation $[\mathbb{Q},\widehat{\rho}_\beta\otimes\widehat{\sigma}] = 0$. The relation (3.11) shows that the above gradient structure leads indeed to DBC Lindbladians. A direct corollary of the above gradient structure are the Onsager operators for the building blocks $\mathcal{M}^\beta_Q$ introduced in Proposition 2.2.

Corollary 3.6 (Simple Onsager operators) *For H and $\widehat{\rho}_\beta$ as above and $(\omega,Q)\in\mathfrak{E}(H)$, we define $\mathcal{K}^\beta_Q(\rho) : \operatorname{Herm}(\mathfrak{h}) \to \operatorname{Herm}(\mathfrak{h})$ and $\mathcal{R}^*_{\beta,Q} : \operatorname{Herm}(\mathfrak{h}) \to [0,\infty[$ as follows:*

$$\mathcal{K}^\beta_Q(\rho)\xi := \big[Q^*,\mathcal{D}^{-\beta\omega}_\rho[Q,\xi]\big] + \big[Q,\mathcal{D}^{\beta\omega}_\rho[Q^*,\xi]\big]$$

Then $\mathcal{K}^\beta_Q$ is an Onsager operator as in Proposition 3.5 and satisfies the identity

$$\mathcal{M}^\beta_Q\rho = -\mathcal{K}^\beta_Q(\rho)\big(\log\rho + \beta H\big) \tag{3.12}$$

Proof: Choose

$$\mathbb{Q} = \begin{pmatrix} 0 & Q^* \\ Q & 0 \end{pmatrix} \quad \widehat{\sigma} = \begin{pmatrix} \mathrm{e}^{\beta\omega/2} & 0 \\ 0 & \mathrm{e}^{-\beta\omega/2} \end{pmatrix}.$$

Then equation (3.12) follows directly from (3.11) and Lemma 3.3. ∎

Our main result concerning the representation of general DBC Lindbladians is now simply stated by collecting the previous results. We have two forms, the first is based on the compact tensor representation and the second is based on the additive form $\mathcal{L} = \sum_{m=1}^{M} \mathcal{M}^{\beta}_{Q_m}$ in terms of the building blocks $\mathcal{M}^{\beta}_{Q_m}$, which will be reflected in an additive structure for the Onsager operator $\mathbb{K}$, whereas the relative entropy as the driving functional is independent of the M different dissipative mechanisms.

Theorem 3.7 (Gradient structure for $\mathcal{L}$ with DBC) *Consider $H \in \mathrm{Herm}(\mathfrak{h})$ and $\widehat{\rho}_\beta$ as above. Then, for any Lindblad operator $\mathcal{L}$ satisfying the DBC* (2.4) *there exists an Onsager operator $\mathbb{K}$ such that $\mathcal{L}$ can be written as $\mathbb{K}$-gradient of the relative entropy $\mathcal{F}_\beta = \mathcal{H}(\cdot|\widehat{\rho}_\beta)$.*
(1) If $\mathcal{L}\rho = -\operatorname{Tr}_{\mathfrak{h}_2}\big([\mathbb{Q},[\mathbb{Q},\rho\otimes\widehat{\rho}_\beta]] = -\operatorname{Tr}_{\mathfrak{h}_2}\big([\widetilde{\mathbb{Q}},[\widetilde{\mathbb{Q}},\rho\otimes\widehat{\rho}_\beta^{-1}]]$ with $\widetilde{\mathbb{Q}} = \mathcal{Y}_{\widehat{\rho}_\beta}\mathbb{Q}$, we can choose

$$\mathbb{K}(\rho)\xi = \operatorname{Tr}_{\mathfrak{h}_2}\Big(\big[\mathbb{Q},\mathcal{C}_{\rho\otimes\widehat{\rho}_\beta}[\mathbb{Q},\xi\otimes\mathbf{1}_{\mathfrak{h}_2}]\big]\Big) \;=\; \operatorname{Tr}_{\mathfrak{h}_2}\Big(\big[\widetilde{\mathbb{Q}},\mathcal{C}_{\rho\otimes\widehat{\rho}_\beta^{-1}}[\widetilde{\mathbb{Q}},\xi\otimes\mathbf{1}_{\mathfrak{h}_2}]\big]\Big).$$

(2) If $\mathcal{L} = \sum_{m=1}^{M} \mathcal{M}^{\beta}_{Q_m}$ with $(\omega_m, Q_m) \in \mathfrak{E}(H)$, we can choose $\mathbb{K}(\rho) = \sum_{m=1}^{M} \mathcal{K}^{\beta}_{Q_m}(\rho)$.

Proof: The result (1) follows by combining the tensor representation in Theorem 2.7 and Proposition 3.5. The result (2) follows by combining the additive representation in Proposition 2.2(c) and Corollary 3.6. ∎

4 Dissipative quantum mechanics via GENERIC

GENERIC is an acronym for General Equations for Non-Equilibrium Reversible Irreversible Coupling, which was introduced by Öttinger and Grmela in [GrÖ97, ÖtG97]. It describes a thermodynamically consistent way of coupling Hamiltonian (=reversible) dynamics with gradient-flow (irreversible) dynamics. It is a variant of metriplectic systems introduced in [Mor84, Mor86], see also [Mor09]. We refer to [MiT16] for an introductory survey of this framework and applications in a large variety of applications. After our general introduction in Section 4.1 we will mainly dwell on the quantum mechanical papers [Ött10, Ött11, Mie13a].

4.1 General setup of GENERIC

A GENERIC system is defined in terms of a quintuple $(\boldsymbol{Q}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$, where the smooth functionals $\mathcal{E}$ and $\mathcal{S}$ on the state space $\boldsymbol{Q}$ denote the total energy and the total entropy, respectively. Moreover, $\boldsymbol{Q}$ carries two geometric structure, namely a Poisson structure $\mathbb{J}$ and a dissipative structure $\mathbb{K}$, i.e., for each $q \in \boldsymbol{Q}$ the operators $\mathbb{J}(q)$ and $\mathbb{K}(q)$ map the cotangent space $\mathrm{T}^*_q\boldsymbol{Q}$ into the tangent space $\mathrm{T}_q\boldsymbol{Q}$. The evolution of the system is given by the differential equation

$$\dot{q} = \mathbb{J}(q)\mathrm{D}\mathcal{E}(q) + \mathbb{K}(q)\mathrm{D}\mathcal{S}(q), \tag{4.1}$$

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

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

$$\mathbb{J}(q) = -\mathbb{J}(q)^* \text{ and } \mathbb{K}(q) = \mathbb{K}(q)^* \tag{4.2a}$$

and the structural properties

$$\begin{aligned} &\mathbb{J} \text{ satisfies Jacobi's identity,} \\ &\mathbb{K}(q) \text{ is positive semi-definite, i.e., } \langle \xi, \mathbb{K}(q)\xi \rangle \geq 0. \end{aligned} \tag{4.2b}$$

Thus, the triples $(\boldsymbol{Q}, \mathcal{E}, \mathbb{J})$ and $(\boldsymbol{Q}, \mathcal{S}, \mathbb{K})$ form a Hamiltonian and an Onsager or gradient system, respectively, with evolution equations $\dot{q} = \mathbb{J}(q)\mathrm{D}\mathcal{E}(q)$ and $\dot{q} = \mathbb{K}(q)\mathrm{D}\mathcal{S}(q)$, respectively. 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)***:

$$\forall\, q \in \boldsymbol{Q}: \quad \mathbb{J}(q)\mathrm{D}\mathcal{S}(q) = 0 \quad \text{and} \quad \mathbb{K}(q)\mathrm{D}\mathcal{E}(q) = 0. \tag{4.2c}$$

A first observation is that (4.2) implies energy conservation and entropy increase:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(q(t)) = \langle \mathrm{D}\mathcal{E}(q), \dot{q} \rangle = \langle \mathrm{D}\mathcal{E}(q), \mathbb{J}\mathrm{D}\mathcal{E} + \mathbb{K}\mathrm{D}\mathcal{S} \rangle = 0 + 0 = 0, \tag{4.3}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(q(t)) = \langle \mathrm{D}\mathcal{S}(q), \dot{q} \rangle = \langle \mathrm{D}\mathcal{S}(q), \mathbb{J}\mathrm{D}\mathcal{E} + \mathbb{K}\mathrm{D}\mathcal{S} \rangle = 0 + \langle \mathrm{D}\mathcal{S}, \mathbb{K}\mathrm{D}\mathcal{S} \rangle \geq 0. \tag{4.4}$$

Note that we would need much less than the three conditions (4.2) to guarantee these two properties. However, the next property needs (4.2c) in its full strength.

Namely 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 $\lambda_{\mathrm{eq}} \neq 0$ we immediately find that x_{eq} is an equilibrium of (4.1). Indeed,

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

where we used the NIC (4.2c).

Vice versa, for every steady state q_{eq} of (4.1) we must have

$$\mathbb{J}(q_{\mathrm{eq}})\mathrm{D}\mathcal{E}(q_{\mathrm{eq}}) = 0 \text{ and } \mathbb{K}(q_{\mathrm{eq}})\mathrm{D}\mathcal{S}(q_{\mathrm{eq}}) = 0. \tag{4.5}$$

Thus, in a steady state there cannot be any balancing between reversible and irreversible forces, both have to vanish independently. To see this we recall the entropy production relation (4.4), which implies $\langle \mathrm{D}\mathcal{S}(q_{\mathrm{eq}}), \mathbb{K}(q_{\mathrm{eq}})\mathrm{D}\mathcal{S}(q_{\mathrm{eq}}) \rangle = 0$ for any steady state. Since $\mathbb{K}(q_{\mathrm{eq}})$ is positive semidefinite, this implies the second identity in (4.5). The first identity then follows from $\dot{q} \equiv 0$ in (4.1).

Very often one is only interested in isothermal systems with fixed temperature $\theta_* > 0$, where the free energy $\mathcal{F}(q) = \mathcal{E}(q) - \theta_*\mathcal{S}(q)$ is a Liapunov function. The associated structure is then that of a damped Hamiltonian system, namely

$$\dot{q} = \Big(\mathbb{J}(q) - \frac{1}{\theta_*}\mathbb{K}(q)\Big)\mathrm{D}\mathcal{F}(q), \tag{4.6}$$

where again $\mathbb{J}$ and $\mathbb{K}$ are Poisson and Onsager structures, respectively. However, there are no longer any non-interaction conditions, since only one functional $\mathcal{F}$ is left.

As in [Mie11a, DPZ13] we note that (4.6) can be converted to a GENERIC system by introducing a scalar slack variable e and defining $\widetilde{\mathcal{E}}(q,e) = \mathcal{F}(q) + e$, $\widetilde{\mathcal{S}}(q,e) = \frac{e}{\theta_*}$,

$$\widetilde{\mathbb{J}}(q,e) = \begin{pmatrix} \mathbb{J}(q) & 0 \\ 0 & 0 \end{pmatrix}, \quad \text{and} \quad \widetilde{\mathbb{K}}(q,e) = \begin{pmatrix} \mathbb{K} & -\mathbb{K}\mathrm{D}\mathcal{F} \\ -(\mathbb{K}\mathrm{D}\mathcal{F})^\top & \langle \mathrm{D}\mathcal{F}, \mathbb{K}\mathrm{D}\mathcal{F}\rangle \end{pmatrix}.$$

Clearly, the NIC (4.2c) are satisfied. The variable e can be seen as the entropic part of the energy. Of course, in concrete cases it is usually easy to find a physically more reasonable splitting into entropy and energy.

4.2 Coupling a dissipative and a quantum system

Since GENERIC systems are closed systems with energy conservation and entropy increase, we need to model all couplings to the quantum system by suitable macroscopic variables. For this aim we introduce the macroscopic variables z lying in a Hilbert space Z. The macro-variable z may include Hamiltonian parts (like the Maxwell equations) as well as dissipative parts producing entropy. The important point of this work is the thermodynamically consistent coupling of the macroscopic system to the quantum system in such a way that energy can be exchanged via Lindblad-like terms.

Following [Ött10, Ött11, Mie13a] we consider an energy and an entropy in the decoupled form

$$\mathcal{E}(\rho,z) = \mathrm{Tr}(\rho H) + E(z) \quad \text{and} \quad \mathcal{S}(\rho,z) = -k_\mathrm{B}\,\mathrm{Tr}(\rho\log\rho) + S(z). \tag{4.7}$$

Whenever suitable we abbreviate the full state with $q = (\rho, z)$ and choose a Poisson structure as follows. Consider a constant macroscopic Poisson operator $\mathbb{J}_\mathrm{ma}(z) : Z^* \to Z$ and a constant coupling operator $\Gamma : L(\mathfrak{h}) \to Z$, then

$$\mathbb{J}(q) = \begin{pmatrix} \mathbb{J}_\mathrm{qs}(\rho) & -\mathbb{J}_\mathrm{qs}(\rho)\Gamma^* \\ -\Gamma\mathbb{J}_\mathrm{qs}(\rho) & \mathbb{J}_\mathrm{ma}{+}\Gamma\mathbb{J}_\mathrm{qs}(\rho)\Gamma^* \end{pmatrix} \text{ with } \mathbb{J}_\mathrm{qs}(\rho)\mu = \mathrm{i}[\rho,\mu], \tag{4.8}$$

is a Poisson structure, which easily follows by transforming the decoupled structure $\mathrm{diag}(\mathbb{J}_\mathrm{qs}, \mathbb{J}_\mathrm{ma})$ via the linear mapping $(\rho,z) \mapsto (\rho, z{-}\Gamma\rho)$.

Using the relation $\mathrm{D}\mathcal{S}(q) = (-k_\mathrm{B}\log\rho, \mathrm{D}_z S(z))$ and $[\rho, \log\rho] = 0$, the first NIC $\mathbb{J}(q)\mathrm{D}\mathcal{S}(q) \equiv 0$ follows by asking

$$\mathbb{J}_\mathrm{ma}(z)\mathrm{D}_z S(z) \equiv 0 \quad \text{and} \quad \Gamma^*\mathrm{D}_z S(z) \equiv 0. \tag{4.9}$$

The choice for the Onsager operator $\mathbb{K}$ is more delicate, since we do not want to generate nonlinear (non-smooth) terms arising from $-k_\mathrm{B}\log\rho$ in the term $\mathbb{K}(q)\mathrm{D}\mathcal{S}(q)$. This will be achieved by using the theory from above concerning the gradient structures for the Lindblad equation for a fixed quantum Hamiltonian H and coupling operators Q_c, where $c \in C$ is a finite set of couplings. Throughout we assume that $(\omega_c, Q_c) \in \mathfrak{E}(H)$ are fixed, while the inverse coupling temperatures $\beta_c(z)$ may depend on the state of the macroscopic system.

More precisely we use the ansatz

$$\begin{aligned} \mathcal{P}^*(\rho, z\,;\, \mu, \zeta) = {}& \frac{1}{2}\langle \zeta\,,\, \mathbb{K}_\mathrm{ma}(z)\zeta\rangle_Z \\ & + \sum_{c\in C} \frac{1}{2} \langle\!\langle\, \mu{-}\langle\zeta, b_c(z)\rangle H \,\|\, \widehat{\mathbb{K}}_c(z)\big(\mu{-}\langle\zeta, b_c(z)\rangle H\big) \,\rangle\!\rangle. \end{aligned} \tag{4.10}$$

for the dual entropy-production potential of the coupled system. Here $\mathbb{K}_{\rm ma}(z) : Z^* \to Z$ is a symmetric and positive semi-definite macroscopic Onsager operator. The coupling vectors $b_c(z) \in Z$ are chosen to satisfy the conditions

$$\forall\, c \in C\, \forall\, z \in Z : \quad \langle \mathrm{D}_z E(z), b_c(z)\rangle_Z = 1 \text{ and } \langle \mathrm{D}_z S(z), b_c(z)\rangle_Z > 0 \tag{4.11}$$

where the first ensures the NIC $\mathbb{K}(\rho, z)\mathrm{D}\mathcal{E}(\rho, z) \equiv 0$ and the second the positivity of the temperature. The Onsager operators $\widehat{\mathbb{K}}_c(z)$, which couple the quantum system via the vector b_c to the macroscopic system, are constructed with the help of the operators $\mathcal{K}^\beta_Q(\rho) : L(\mathfrak{h}) \to L(\mathfrak{h})$ from Corollary 3.6 as follows:

$$\widehat{\mathbb{K}}_c(z) = \kappa_c(z)\mathcal{K}^{\widehat{\beta}_c(z)}_{Q_c}(\rho), \quad \text{where } \widehat{\beta}_c(z) := \frac{1}{k_{\rm B}}\langle \mathrm{D}_z S(z), b_c(z)\rangle_Z \text{ and } \kappa_c(z) \geq 0. \tag{4.12}$$

Hence, the full Onsager operator takes the form

$$\mathbb{K}(q) = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{K}_{\rm ma}(z) \end{pmatrix} + \sum_{c\in C} \begin{pmatrix} \widehat{\mathbb{K}}_c & -\langle \Box, b_c\rangle_Z \widehat{\mathbb{K}}_c H \\ -\langle\!\langle H \,\|\, \widehat{\mathbb{K}}_c \Box \rangle\!\rangle b_c & \langle\!\langle H \,\|\, \widehat{\mathbb{K}}_c H \rangle\!\rangle b_c \otimes b_c \end{pmatrix}, \tag{4.13}$$

where $\Box$ indicates where the corresponding argument has to be inserted. Using the definition of $\widehat{\beta}_c$ in (4.12) we easily see that the NIC $\mathbb{K}(\rho, z)\mathrm{D}\mathcal{E}(\rho, z) \equiv 0$ holds, if we assume $\mathbb{K}_{\rm ma}(z)\mathrm{D}_z E(z) \equiv 0$. We emphasize that $\mathbb{K}$ depends highly nonlinearly on ρ through $\mathcal{K}^{\beta_c(z)}_{Q_c}(\rho)$, which in turn depends on $\mathcal{D}^{\pm\widehat{\beta}_c(z)\omega_c}_\rho$.

Proposition 4.1 (GENERIC structure) *Let $X = \mathfrak{R} \times Z$ and let $\mathcal{E}$ and $\mathcal{S}$ be given in the decoupled form* (4.7)*. Moreover, consider the Poisson structure $\mathbb{J}$ defined in* (4.8) *and the Onsager structure $\mathbb{K}$ defined in* (4.13)*. Assuming additionally* (4.11)*, $\mathbb{J}_{\rm ma}\mathrm{D}S \equiv 0$, $\Gamma^*\mathrm{D}S \equiv 0$, and $\mathbb{K}_{\rm ma}\mathrm{D}E \equiv 0$ the quintuple $(X, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$ forms a GENERIC system.*

So far, we have not used the special form of $\widehat{\mathbb{K}}_c$ defined in terms of $\mathcal{K}^{\beta_c}_{Q_c}$. The advantage of this choice is of course dictated by the aim to obtain a linear Lindblad equation for ρ. Indeed, using the relation (3.12) relating $\mathcal{K}^\beta_Q$ and $\mathcal{M}^\beta_Q$ we see that the equations obtained from the GENERIC system have the explicit form

$$\begin{aligned} \begin{pmatrix} \dot\rho \\ \dot z \end{pmatrix} &= \mathbb{J}(\rho, z)\mathrm{D}\mathcal{E}(\rho, z) + \mathbb{K}(\rho, z)\mathrm{D}\mathcal{S}(\rho, z) \\ &= \begin{pmatrix} \mathbb{J}_{\rm qs}(\rho) & -\mathbb{J}_{\rm qs}(\rho)\Gamma^* \\ -\Gamma\mathbb{J}_{\rm qs}(\rho) & \mathbb{J}_{\rm ma} + \Gamma\mathbb{J}_{\rm qs}(\rho)\Gamma^* \end{pmatrix} \begin{pmatrix} H \\ \mathrm{D}E(z) \end{pmatrix} + \begin{pmatrix} 0 \\ \mathbb{K}_{\rm ma}(z)\mathrm{D}S(z) \end{pmatrix} \\ &\quad + \sum_{c\in C} \begin{pmatrix} \widehat{\mathbb{K}}_c & -\langle \Box, b_c\rangle_Z \widehat{\mathbb{K}}_c H \\ -\langle\!\langle H \,\|\, \widehat{\mathbb{K}}_c \Box \rangle\!\rangle b_c & \langle\!\langle H \,\|\, \widehat{\mathbb{K}}_c H \rangle\!\rangle b_c \otimes b_c \end{pmatrix} \begin{pmatrix} -k_{\rm B}\log\rho \\ \mathrm{D}S(z) \end{pmatrix}. \end{aligned} \tag{4.14}$$

Introducing the effective Hamiltonian $\widetilde{H}(z)$ through

$$\widetilde{H}(z) = H - \Gamma^*\mathrm{D}E(z).$$

and using the construction of $\widehat{\mathbb{K}}_c(\rho, z)$ via $\mathcal{K}^{\widehat{\beta}_c(z)}_{Q_c}(\rho)$ we arrive at a coupled system for ρ and z that is indeed linear in ρ, namely

$$\begin{aligned} \begin{pmatrix} \dot\rho \\ \dot z \end{pmatrix} = \begin{pmatrix} \mathrm{i}\big[\rho\,,\, \widetilde{H}(z)\big] \\ \mathbb{J}_{\rm ma}\mathrm{D}E(z) - \mathrm{i}\Gamma\big[\rho\,,\, \widetilde{H}(z)\big] \end{pmatrix} + \begin{pmatrix} 0 \\ \mathbb{K}_{\rm ma}(z)\mathrm{D}S(z) \end{pmatrix} \\ + \sum_{c\in C} \begin{pmatrix} k_{\rm B}\kappa_c(z)\mathcal{M}^{\beta_c(z)}_{Q_c}\rho \\ -k_{\rm B}\kappa_c(z)\langle\!\langle H \,\|\, \mathcal{M}^{\beta_c(z)}_{Q_c}\rho \rangle\!\rangle b_c(z) \end{pmatrix}. \end{aligned} \tag{4.15}$$

Moreover, the coupling of the linear quantum system for ρ with the macroscopic system for z is given in a very particular manner reflecting the DBC, as the vectors $b_c(z)$ occur twice, namely (i) in the definition of $\beta_c(z) = \langle \mathrm{D}S(z), b_c(z)\rangle / k_\mathrm{B}$ in (4.12) and (ii) in the equation for z, i.e. the second component of (4.15). The fact that this equation is obtained from the GENERIC system $(\mathfrak{R} \times Z, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$ implies energy conservation and entropy production along solutions $q(t) = (\rho(t), z(t))$, namely $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(q(t)) \equiv 0$ and

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(q(t)) &= 2\mathcal{P}^*(q(t), \mathrm{D}\mathcal{S}(t)) \\ &= 2\langle \mathrm{D}S, \mathbb{K}_\mathrm{ma}\mathrm{D}S\rangle_Z + 2k_\mathrm{B}^2 \sum_{c\in C} \langle\!\langle \log\rho + \widehat{\beta}_c H \,\|\, \mathcal{K}_{Q_c}^{\widehat{\beta}_c}(\log\rho + \widehat{\beta}_c H) \rangle\!\rangle \geq 0.\end{aligned}$$

5 Examples and applications

We discuss the above construction and give a few examples and applications to highlight the concept of the operators $\mathcal{D}_\rho^\alpha$ and the relevance of the corresponding Lindblad operators. From a modeling point of view, we emphasize that using the gradient structure with respect to the relative entropy, it is easy to construct thermodynamically consistent coupled system including macroscopic variables $z \in Z$ and a quantum state ρ, see e.g. the quantum-dot model discussed in Section 5.4. In particular, we can interprete the dissipative mechanisms in the macroscopic system and in the quantum system as given building blocks that have to be combined in a suitable way to obtain a thermodynamically correct system. This can either be a damped Hamiltonian system at constant temperature or a GENERIC (General Equation for Non-Equilibrium Reversible Irreversible Coupling) system where the total energy is preserved while the physical entropy increases.

5.1 The isothermal, damped quantum system

For a general DBC Lindbladian $\mathcal{L}$ with respect to $\widehat{\rho}_\beta = \frac{1}{Z}\mathrm{e}^{-\beta H}$ Proposition 2.2 shows that it can be written as a sum of operators $\mathcal{M}_Q^\beta$ as defined in Proposition 2.2(b). Indeed, we have

$$\dot\rho = \mathrm{i}[\rho, H] + \mathcal{L}\rho = \mathrm{i}[\rho, H] + \sum_{c\in C} \mathcal{M}_{Q_c}^\beta \rho, \tag{5.1}$$

where the coupling operator Q_c satisfy $(\omega_c, Q_c) \in \mathfrak{E}(H)$.

We are now able to state that all dissipative quantum generators satisfying the DBC can be written as a damped Hamiltonian system $(\mathfrak{R}, \mathcal{F}, \mathbb{J}, \mathbb{K})$, namely

$$\dot\rho = \mathrm{i}[\rho, H] + \mathcal{L}\rho = \big(\mathbb{J}_\mathrm{qs}(\rho) - \mathbb{K}(\rho)\big)\mathrm{D}\mathcal{F}(\rho),$$

where we can use the following choices

$$\mathcal{F}(\rho) = \mathrm{Tr}\,\big(\beta H + \rho\log\rho\big), \quad \mathbb{J}_\mathrm{qs}(\rho) = \mathrm{i}\big[\rho, \Box\big], \quad \text{and} \quad \mathbb{K}(\rho) = \sum_{c\in C} \mathcal{K}_{Q_c}^\beta(\rho).$$

For this we simply use that $(\omega, Q) \in \mathfrak{E}(H)$ implies $\mathcal{K}_Q^\beta(\log\rho + \beta H) = \mathcal{M}_Q^\beta \rho$, see (3.12).

5.2 Coupling to simple heat baths

We consider a quantum system coupled to a finite number of finite-energy heat baths indexed by $m = 1, .., M$. We set $Z = \mathbb{R}^M$ with elements $z = \boldsymbol{\theta} = (\theta_m)_m$, where $\theta_m > 0$ denotes the absolute temperature of the mth heat bath. Each heat bath is coupled to the quantum state ρ such that energy may flow from one heat bath into the others via the quatum system.

We assume each heat bath to have a constant specific heat c_m. Hence, we let

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

For the coupling vectors b_m we choose

$$b_m(\boldsymbol{\theta}) = \frac{1}{c_m} \boldsymbol{e}^{(m)} \in \mathbb{R}^M, \quad \text{where } \boldsymbol{e}^{(m)} = (0, .., 0, 1, 0, .., 0)^\top$$

is the mth unit vector. Clearly we find

$$b_m(\boldsymbol{\theta}) \cdot \mathrm{D}E(\boldsymbol{\theta}) \equiv 1 \quad \text{and} \quad \widehat{\beta}_m(\boldsymbol{\theta}) = \frac{1}{k_\mathrm{B}} b_m(\boldsymbol{\theta}) \cdot \mathrm{D}S(\boldsymbol{\theta}) = \frac{1}{k_\mathrm{B}\theta_m},$$

which is the usual inverse temperature of the mth heat bath.

Assuming $\mathbb{J}_\mathrm{ma} \equiv 0$ and $\Gamma = 0$, we can choose a symmetric and positive semi-definite matrix $K_\mathrm{ma} \in \mathbb{R}^{M\times M}$ such that $K_\mathrm{ma}\overline{\boldsymbol{c}} = 0$, where $\overline{\boldsymbol{c}}$ is the constant vector $\mathrm{D}E(\boldsymbol{\theta}) = (1/c_m)_{m=1,..,M}$. The construction in Section 4.2 provides a GENERIC system for $q = (\rho, \boldsymbol{\theta})$ in the following form:

$$\begin{aligned} \dot\rho &= \mathrm{i}[\rho, H] + \sum_{m=1}^{M} \mathcal{M}_{Q_m}^{1/(k_\mathrm{B}\theta_m)} \rho, \\ \dot{\boldsymbol{\theta}} &= K_\mathrm{ma} \mathrm{D}S(\boldsymbol{\theta}) + \sum_{m=1}^{M} \frac{1}{c_m} \langle\!\langle\, H \,\|\, \mathcal{M}_{Q_m}^{1/(k_\mathrm{B}\theta_m)} \rho \,\rangle\!\rangle\, \boldsymbol{e}^{(m)}. \end{aligned} \tag{5.2}$$

It is now easy to see that we may take the heat capacities very large, such that the temperatures θ_m do not change any more, or at least not on the time scale where the typical changes of ρ occur. Thus, it is possible to investigate in a natural way non-equilibrium steady states, where energy is exchanged between heat baths with different temperatures.

5.3 An isothermally coupled system

Here we return to an isothermally system where the quantum state ρ is coupled to a macroscopic variable z in such a way that we obtain a damped Hamiltonian system. In contrast to the simple model in Section 5.1 we now allow the effective inverse temperatures $\widehat{\beta}_c$ to depend on the state z. Here we give a general form of such systems and in Section 5.4 we provide a model for a quantum dot interaction with charge-carrier densities taking the roles of z.

For the definition of the free energy $\mathcal{F}$ we choose the fixed equilibrium temperature θ_* and obtain

$$\mathcal{F}(\rho, z) = \frac{1}{k_\mathrm{B}\theta_*} \mathcal{E}(\rho, z) - \frac{1}{k_\mathrm{B}} \mathcal{S}(\rho, z) = \mathrm{Tr}\left(\rho \log \rho + \frac{1}{k_\mathrm{B}\theta_*} \rho H\right) + F(z).$$

We may take $\mathbb{J}$ as in (4.8) but need to choose a special $\mathbb{K}$ to obtain equations linear in ρ, namely

$$\mathbb{K}(\rho,z)=\begin{pmatrix}0&0\\0&\mathbb{K}_{\mathrm{ma}}(z)\end{pmatrix}+\sum_{c\in C}\begin{pmatrix}\widetilde{\mathbb{K}}_c & \langle\Box,a_c\rangle_Z\,\widetilde{\mathbb{K}}_cH\\ \langle\!\langle\, H\,\|\,\widetilde{\mathbb{K}}_c\Box\,\rangle\!\rangle a_c & \langle\!\langle\, H\,\|\,\widetilde{\mathbb{K}}_cH\,\rangle\!\rangle a_c\otimes a_c\end{pmatrix}$$

with coupling vectors $a_c(z)\in Z$ and Onsager operators $\widetilde{\mathbb{K}}_c(\rho,z)=\kappa_c(z)\mathcal{K}_{Q_c}^{\widetilde{\beta}_c(z)}(\rho)$, where

$$\kappa_c(z)\geq 0\quad\text{and}\quad\widetilde{\beta}_c(z)=\frac{1}{k_{\mathrm{B}}\theta_*}+\langle\mathrm{D}F(z),a_c(z)\rangle_Z>0.$$

Hence, the equations $\dot q=\big(\mathbb{J}(q)-\mathbb{K}(q)\big)\mathrm{D}\mathcal{F}(q)$ take the form

$$\begin{aligned}\dot\rho&=\mathrm{i}\big[\rho,H-\Gamma^*\mathrm{D}F(z)\big] && +\sum_{c\in C}\kappa_c(z)\mathcal{M}_{Q_c}^{\widetilde{\beta}_c(z)}\rho,\\ \dot z&=\mathbb{J}_{\mathrm{ma}}\mathrm{D}F(z)-\mathrm{i}\Gamma\big[\rho,H-\Gamma^*\mathrm{D}F(z)\big] && +\sum_{c\in C}\kappa_c(z)\langle\!\langle\, H\,\|\,\mathcal{M}_{Q_c}^{\widetilde{\beta}_c(z)}\rho\,\rangle\!\rangle a_c(z).\end{aligned}$$

Again $F(Z)$, $a_c(z)$, and $\widetilde{\beta}_c(z)$ are intrinsically linked to each other in order to generate this evolutionary equation from the damped Hamiltonian system $(\mathfrak{R}\times Z,\mathcal{F},\mathbb{J},\mathbb{K})$.

5.4 A quantum dot interacting with charge carriers

In [RG*10] a four-level model with two levels in the conduction and two levels in the valence band is described in detail. However, the charge carriers in the wetting layer are assumed to be given, i.e. kept constant during the experiment. In [LMS09], the turn-on behavior of single quantum-dot lasers was analyzed based on a rate equation for the photon density n_{ph}, the densities w_{e} and w_{h} for electrons and holes in the wetting layer, and the charge carriers n_{e} and n_{h} in the quantum dot. We will show in [MMR17] that the approach developed in Section 5.3 allows us to combine theses two approaches to derive a thermodynamically consistent model coupling the charge-carrier relaxation with the state of the quantum dot.

Here we look at a very simplistic model, where the quantum system has only two states with energies $\varepsilon_2>\varepsilon_1$. Moreover, in the wetting layer we have free charge carriers with density c_{f} that can be captured by the quantum dot leading to a density c_{b} of bound charge carriers. This charge capture excites the quantum state from $|1\rangle$ to $|2\rangle$:

$$X_{\text{free}}+|1\rangle\quad\rightleftharpoons\quad X_{\text{bound}}+|2\rangle.$$

This is one example of several capture-escape or scattering processes that need to be modeled for a complete description of single quantum-dot lasers, see [RG*10].

With $H=\mathrm{diag}(\varepsilon_1,\varepsilon_2)\in\mathrm{Herm}(\mathbb{C}^2)$, a fixed $\beta_*>0$, and the density vector $z=\boldsymbol{c}=(c_{\mathrm{f}},c_{\mathrm{b}})\in\,]0,\infty[^2$, we have the relative entropy

$$\mathcal{F}(\rho,z)=\mathrm{Tr}(\rho\log\rho+\beta_*\rho H)+c_{\mathrm{f}}\big(\log(c_{\mathrm{f}}/w_{\mathrm{f}})-1\big)+c_{\mathrm{b}}\big(\log(c_{\mathrm{b}}/w_{\mathrm{b}})-1\big),$$

where $w_{\mathrm{f}},w_{\mathrm{b}}>0$ are suitable equilibrium densities. With

$$\boldsymbol{a}=\frac{1}{\varepsilon_2-\varepsilon_1}\begin{pmatrix}-1\\1\end{pmatrix}\ \text{ and }\ Q=|1\rangle\langle 2|=\begin{pmatrix}0&1\\0&0\end{pmatrix}$$

we define the Onsager operator as in Section 5.3:

$$\mathbb{K}(\rho,\boldsymbol{c})=\kappa(\boldsymbol{c})\begin{pmatrix} \mathcal{K}_Q^{\widetilde\beta(\boldsymbol{c})}(\rho) & \langle \boldsymbol{a},\Box\rangle_Z\,\mathcal{K}_Q^{\widetilde\beta(\boldsymbol{c})}(\rho)H \\ \langle\!\langle\, H\,\|\,\mathcal{K}_Q^{\widetilde\beta(\boldsymbol{c})}(\rho)\Box\,\rangle\!\rangle\boldsymbol{a} & \langle\!\langle\, H\,\|\,\mathcal{K}_Q^{\widetilde\beta(\boldsymbol{c})}(\rho)H\,\rangle\!\rangle\boldsymbol{a}\otimes\boldsymbol{a}\end{pmatrix},$$

where $\kappa(\boldsymbol{c})=\widehat\kappa\big(\frac{c_\mathrm{f}c_\mathrm{b}}{w_\mathrm{f}w_\mathrm{b}}\big)^{1/2}$ and $\widetilde\beta(\boldsymbol{c})=\beta_*-\dfrac{1}{\varepsilon_2{-}\varepsilon_1}\big(\log(c_\mathrm{f}/w_\mathrm{f})-\log(c_\mathrm{b}/w_\mathrm{b})\big)$.

Here $\widetilde\beta(\boldsymbol{c})$ and $\boldsymbol{a}$ are chosen in a very particular way such that

$$\begin{aligned} &-\mathbb{K}(\rho,\boldsymbol{c})\mathrm{D}\mathcal{F}(\rho,\boldsymbol{c})=-\mathbb{K}(\rho,\boldsymbol{c})\begin{pmatrix}\log\rho+\beta_*H\\ (\log c_j/a_j)_{j\in\{\mathrm{f},\mathrm{b}\}}\end{pmatrix}\\ &=-\kappa(\boldsymbol{c})\begin{pmatrix}\mathcal{K}_Q^{\widetilde\beta(\boldsymbol{c})}(\rho)\big(\log\rho+\widetilde\beta(\boldsymbol{c})H\big)\\ \langle\!\langle\, H\,\|\,\mathcal{K}_Q^{\widetilde\beta(\boldsymbol{c})}(\rho)\big(\log\rho+\widetilde\beta(\boldsymbol{c})H\big)\,\rangle\!\rangle\boldsymbol{a}\end{pmatrix}=\kappa(\boldsymbol{c})\begin{pmatrix}\mathcal{M}_Q^{\widetilde\beta(\boldsymbol{c})}\rho\\ \langle\!\langle\, H\,\|\,\mathcal{M}_Q^{\widetilde\beta(\boldsymbol{c})}\rho\,\rangle\!\rangle\boldsymbol{a}\end{pmatrix},\end{aligned}$$

where we used the miracle identity as stated in Corollary 3.6.

Using the explicit form of $\mathcal{M}_Q^b$, H, Q, and $\widetilde\beta(\boldsymbol{c})$ we obtain (with $\omega=\varepsilon_2{-}\varepsilon_1$)

$$\mathcal{M}_Q^{\widetilde\beta(\boldsymbol{c})}\rho=\mathrm{e}^{\beta_*\omega/2}\big(\frac{c_\mathrm{b}}{a_\mathrm{b}}\frac{a_\mathrm{f}}{c_\mathrm{f}}\big)^{1/2}\mathcal{N}_Q\rho+\mathrm{e}^{-\beta_*\omega/2}\big(\frac{c_\mathrm{f}}{w_\mathrm{f}}\frac{w_\mathrm{b}}{c_\mathrm{b}}\big)^{1/2}\mathcal{N}_{Q^*}\rho\Big),$$

where $\mathcal{N}_QA:=[Q,AQ^*]+[QA,Q^*]$.

By our specific choice of $\kappa(\boldsymbol{c})$ all the square roots cancel, and we see that the final coupled system takes the form (where $\widetilde\kappa=\widehat\kappa\mathrm{e}^{\beta_*(\varepsilon_1+\varepsilon_2)/2}$)

$$\dot\rho \;=\; \mathrm{i}[\rho,H]+\widetilde\kappa\Big(\frac{c_\mathrm{b}}{w_\mathrm{b}}\mathrm{e}^{-\beta_*\varepsilon_1}\mathcal{N}_Q\rho+\frac{c_\mathrm{f}}{w_\mathrm{f}}\mathrm{e}^{-\beta_*\varepsilon_2}\mathcal{N}_{Q^*}\rho\Big), \tag{5.3a}$$

$$\begin{pmatrix}\dot c_\mathrm{f}\\ \dot c_\mathrm{b}\end{pmatrix}=2\widetilde\kappa\left(\frac{c_\mathrm{f}}{w_\mathrm{f}}\mathrm{e}^{-\beta_*\varepsilon_2}\rho_{11}-\frac{c_\mathrm{b}}{w_\mathrm{b}}\mathrm{e}^{-\beta_*\varepsilon_1}\rho_{22}\right)\begin{pmatrix}-1\\ 1\end{pmatrix}, \tag{5.3b}$$

where we used $\langle\!\langle\, H\,\|\,\mathcal{N}_Q\rho\,\rangle\!\rangle=-2\omega\rho_{22}$ and $\langle\!\langle\, H\,\|\,\mathcal{N}_{Q^*}\rho\,\rangle\!\rangle=2\omega\rho_{11}$. Thus, we obtain a coupled system with quadratic nonlinearities.

Since $\mathcal{N}_Q$ and $\mathcal{N}_{Q^*}$ are Lindblad operators, we see that (5.3a) is a Lindblad equation that depends on the macroscopic variables $\boldsymbol{c}=(c_\mathrm{f},c_\mathrm{b})$. The charge carrier densities c_f and c_b are driven by the quantum state ρ in such a way that $c_\mathrm{f},c_\mathrm{b}>0$ is always preserved. The important message of our construction is that this system is a damped Hamiltonian system, and thus the relative entropy $\mathcal{F}$ is a Liapunov function.

5.5 Maxwell-Bloch model

In this section we discuss a nonlinear PDE model, where the Maxwell equations on $\mathbb{R}^3$ as the macroscopic Hamiltonian system are coupled to a spatially localized domain $\Omega\subset\mathbb{R}^3$, where at each macroscopic point $x\in\Omega$ there is a quantum system that is coupled to the electromagnetic fields $\boldsymbol{E}$ and $\boldsymbol{H}$, but not to the neighboring quantum systems. Such models are called Maxwell-Bloch systems (cf. e.g. [JMR00, Dum05]) and are commonly used to model the interaction of light and matter. We refer to [Mie15] where even the coupling to the drift-diffusion system for electrons and holes is described in terms of the GENERIC framework.

The macroscopic system is described by $z = (\boldsymbol{E}, \boldsymbol{H}) \in Z := \mathrm{L}^2(\mathbb{R}^3; \mathbb{R}^3)^2$ denoting the electric and the magnetic fields. The optically active material is described by a bounded Lipschitz domain $\Omega \subset \mathbb{R}^3$, where the quantum state is described via $\rho : \Omega \to \mathfrak{R}_N \subset \mathrm{Herm}(\mathfrak{h})$. The quantum state determines the macroscopic polarization $\boldsymbol{P} : \Omega \to \mathbb{R}^3$ via a polarization operator $\Gamma : L(\mathfrak{h}) \to \mathbb{R}^3$ in the form $\boldsymbol{P}(x) = \Gamma\rho(x)$. The electric displacement field then is given by $\boldsymbol{D} = \varepsilon_0\boldsymbol{E} + \boldsymbol{P}$, and Maxwell equations take the form

$$\varepsilon_0\dot{\boldsymbol{E}} + \dot{\boldsymbol{P}} = \mathrm{curl}\,\boldsymbol{H}, \quad \mu_0\dot{\boldsymbol{H}} = -\,\mathrm{curl}\,\boldsymbol{E}, \quad \mathrm{div}\,\big(\varepsilon_0\boldsymbol{E}+\boldsymbol{P}\big) = 0, \quad \mathrm{div}\,\boldsymbol{H} = 0. \tag{5.4}$$

The main difficulty is to model the coupling of the quantum systems $\rho(t, x) \in \mathfrak{R}_N$ in a consistent way. We derive the system for $q := (\rho, \boldsymbol{E}, \boldsymbol{H})$ in the form of a damped Hamiltonian system with the free energy

$$\mathcal{F}(q) = \int_{\mathbb{R}^d} \frac{1}{2}|\boldsymbol{E}|^2 + \frac{1}{2}|\boldsymbol{H}|^2 \,\mathrm{d}x + \int_\Omega \mathrm{Tr}\,\big(\rho\log\rho + \beta H_{\mathrm{B}}\rho\big)\,\mathrm{d}x,$$

where H_{B} is called the Bloch Hamiltonian and where we have set the constants ε_0 and μ_0 to 1 for notational simplicity. Moreover, we define a Poisson structure $\mathbb{J}$ and an Onsager operator $\mathbb{K}$ in the form

$$\mathbb{J}(q) = \begin{pmatrix} \mathrm{i}[\rho, \Box] & -\mathrm{i}\big[\rho, \Gamma^*\Box\big] & 0 \\ -\mathrm{i}\Gamma\big[\rho, \Box\big] & \mathrm{i}\Gamma\big[\rho, \Gamma^*\Box\big] & \mathrm{curl} \\ 0 & -\,\mathrm{curl} & 0 \end{pmatrix} \text{ and } \mathbb{K}(q) = \begin{pmatrix} \mathbb{K}_{\mathrm{qs}}(q) & -\mathbb{K}_{\mathrm{qs}}(q)\Gamma^* & 0 \\ -\Gamma\mathbb{K}_{\mathrm{qs}}(q) & \Gamma\mathbb{K}_{\mathrm{qs}}(q)\Gamma^* & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The importance of this choice for $\mathbb{J}$ and $\mathbb{K}$ is that the first row of each of the block operators is replicated in the second row, but premultiplied with $-\Gamma$. This is needed to obtain the correct first equation in the Maxwell system (5.4), namely

$$\dot{\boldsymbol{E}} = \mathrm{curl}\,\boldsymbol{H} - \dot{\boldsymbol{P}} = \mathrm{curl}\,\boldsymbol{H} - \Gamma\dot{\rho}.$$

By the symmetries $\mathbb{J} = -\mathbb{J}^*$ and $\mathbb{K} = \mathbb{K}^*$ this also implies that the first columns are replicated in the second columns, but now post-multiplied by $-\Gamma^*$.

We emphasize that the optically active material is restricted to the bounded domain Ω, while the fields $\boldsymbol{E}$ and $\boldsymbol{H}$ are defined on all of $\mathbb{R}^3$. This is hidden in our operator Γ, which should be understood as an operator that maps ρ defined on Ω to vector fields $\boldsymbol{P} = \Gamma\rho$ that are defined not only in Ω, but that are extended by 0 outside of Ω. Similarly, the adjoint operator Γ^* acts on $\boldsymbol{E}$ by restricting it first to Ω and then applying the adjoint map of Γ.

Thus, using $[\rho, \log\rho] = 0$ the induced equation for ρ reads

$$\dot{\rho} \;=\; \mathrm{i}\big[\,\rho,\, \beta H_{\mathrm{B}} - \Gamma^*\boldsymbol{E}\,\big] \;-\; \mathbb{K}_{\mathrm{qs}}(\rho, \boldsymbol{E}, \boldsymbol{H})\big(\log\rho + \beta H_{\mathrm{B}} - \Gamma^*\boldsymbol{E}\big).$$

Having derived this structure it is now our task to choose $\mathbb{K}_{\mathrm{qs}}$ in such a way that the equation for ρ is a Lindblad equation that is linear in ρ with coefficients depending on $\boldsymbol{E}$ and $\boldsymbol{H}$. For this, we assume that there exists a family $(Q_c)_{c\in C}$ of couplings such that

$$(\omega_c, Q_c) \in \mathfrak{E}(H_{\mathrm{B}}) \quad \text{and} \quad [Q_c, \Gamma^*\boldsymbol{E}] = \omega_c\,(\boldsymbol{g}_c{\cdot}\boldsymbol{E})\,Q_c, \tag{5.5}$$

for some vectors $\boldsymbol{g}_c \in \mathbb{R}^3$. Note that this is a non-trivial condition, since it implies that for all $\boldsymbol{E} \in \mathbb{R}^3$ the matrix $\Gamma^*\boldsymbol{E} \in \mathrm{Herm}(\mathfrak{h})$ commutes with all matrices Q that commute with H.

Based on the assumption (5.5) we are now able to choose $\mathbb{K}_{\mathrm{qs}}$ in the form

$$\mathbb{K}_{\mathrm{qs}}(\rho, \boldsymbol{E}, \boldsymbol{H}) = \sum_{c\in C} \kappa_c(\boldsymbol{E}, \boldsymbol{H})\,\mathcal{K}_{Q_c}^{\widetilde{\beta}_c(\boldsymbol{E})}(\rho), \quad \text{where } \widetilde{\beta}_c(\boldsymbol{E}) := \beta - \boldsymbol{g}_c{\cdot}\boldsymbol{E}.$$

Since by construction we have $[Q_c, \beta H_{\mathrm{B}} - \Gamma^* \boldsymbol{E}] = \omega_c \widetilde{\beta}_c(\boldsymbol{E}) Q_c$ we can apply Proposition 3.6 (cf. (3.12)) and obtain the equation

$$\dot{\rho} = \mathrm{i}\big[\,\rho,\, \beta H_{\mathrm{B}} - \Gamma^* \boldsymbol{E}\,\big] + \sum_{c\in C} \kappa_c(\boldsymbol{E}, \boldsymbol{H})\, \mathcal{M}_{Q_c}^{\widetilde{\beta}_c(\boldsymbol{E})} \rho,$$

which is linear in ρ for fixed $\boldsymbol{E}$ and $\boldsymbol{H}$. Note that for the above constructions it is not necessary to have $\widetilde{\beta}_c \geq 0$, since $\mathcal{K}_Q^\beta$ and $\mathcal{M}_Q^\beta$ are well defined for all $\beta \in \mathbb{R}$. Altogether we conclude that under the rather restrictive assumption (5.5) the damped Hamiltonian system $(\mathrm{L}^2(\Omega; \mathfrak{R}_N) \times Z, \mathcal{F}, \mathbb{J}, \mathbb{K})$ generates the following coupled Maxwell-Bloch system

$$\begin{aligned}
\dot{\rho} &= \mathrm{i}\big[\rho, H_{\mathrm{B}} - \Gamma^* \boldsymbol{E}\big] + \sum_{c\in C} \kappa_c(q) \mathcal{M}_{Q_c}^\beta \rho, \\
\dot{\boldsymbol{E}} &= \operatorname{curl} \boldsymbol{H} - \Gamma\Big(\mathrm{i}\big[\rho, H_{\mathrm{B}} - \Gamma^* \boldsymbol{E}\big] + \sum_{c\in C} \kappa_c(q) \mathcal{M}_{Q_c}^\beta \rho\Big), \\
\dot{\boldsymbol{H}} &= -\operatorname{curl} \boldsymbol{E}.
\end{aligned}$$

It is easy to see that condition (5.5) holds, if Γ has the form $\Gamma \boldsymbol{E} = \sum_{n=1}^N (\boldsymbol{b}_n \cdot \boldsymbol{E})\, h_n \otimes \overline{h}_n$ for arbitrary polarization vectors $\boldsymbol{b}_n \in \mathbb{R}^3$, where $H = \sum_1^N \varepsilon_n h_n \otimes \overline{h}_n$. It remains open to model the case of interaction between different energy levels, for which $\Gamma \boldsymbol{E}$ needs to contain terms like $h_m \otimes \overline{h}_n$ with $m \neq n$.

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