Open quantum systems – lecture 15

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5.3 Collective coordinate mappings

Suppose the total Hamiltonian of the universe has the structure of a (possibly semi-infinite) chain, with the system located at the end. To infer the dynamics of the system, i.e., the first (few) site(s), we could derive the master equation for it, which heavily depends on the spectral function of the chain reservoir. To improve the validity of the master equation, we can extend the system by shifting the boundary between system and reservoir along the chain and then compute the master equation for the extended system. Setting up the master equation will require the computation of the spectral function of the residual reservoir, and solving it will require more resources as the system has become larger with this procedure.

In case a chain structure is not provided, i.e., if one starts from a star configuration, one may always reconstruct at least a partial chain structure: A single collective coordinate may then be incorporated into the system, taking the impact of the reservoir into account.

5.3.1 Bosonic mappings

Bosonic Bogoliubov transforms

In a nutshell, Bogoliubov transforms (compare lecture on Advanced Mathematical Methods) map bosonic (or fermionic) creation and annihilation operators to new bosonic (or fermionic) creation and annihilation operators while leaving their (anti-)commutation relations invariant.

Def. 1 (Bosonic Bogoliubov transform)**.** *A bosonic Bogoliubov transform is a linear mapping between bosonic annihilation and creation operators, which preserves the corresponding bosonic commutation relations*

$$a_k = \sum_q \left[u_{kq} b_q + v_{kq} b_q^\dagger\right] , \qquad \begin{aligned} \left[a_k, a_{k'}^\dagger\right] &= \delta_{kk'} , & [a_k, a_{k'}] &= 0 , \\ \left[b_k, b_{k'}^\dagger\right] &= \delta_{kk'} , & [b_k, b_{k'}] &= 0 , \end{aligned} \tag{5.1}$$

where $u_{kq}, v_{kq} \in \mathbb{C}$.

The demand that the commutation relations must be preserved puts additional constraints on the a priori unknown coefficients u_{kq} and v_{kq}. For example, from the commutation relations we obtain the conditions

$$\begin{aligned} \left[a_k, a_{k'}^\dagger\right] &= \sum_q \left(u_{kq} u_{k'q}^* - v_{kq} v_{k'q}^*\right) = \delta_{kk'} , \\ [a_k, a_{k'}] &= \sum_q \left(u_{kq} v_{k'q} - v_{kq} u_{k'q}\right) = 0 , \end{aligned} \tag{5.2}$$

where we note that the equation $\left[a_k^\dagger, a_{k'}^\dagger\right] = 0$ just adds the conjugate of the second constraint.

- A simple but special solution to these equations is to choose $v_{kk'} = 0$. Then, creation and annihilation operators are not mixed, the second of Eq. (5.2) is trivially fulfilled, and the first reduces to a unitarity condition $\sum_q u_{kq} u_{k'q}^* = \delta_{kk'}$ on the matrix formed by the u_{kq}.

In this case, the Bogoliubov transform therefore reduces to a unitary transform between annihilation operators. An even more trivial example of unitary Bogoliubov transforms is the multiplication of the creation and annihilation operators by a phase factor (absence of any mixing): When discussing operator transforms, we noted that time-dependent phase factors would e.g. arise in the interaction picture.

- Another special case is obtained when parametrizing the u_{kq} and v_{kq} by an orthogonal matrix

$$u_{kq} = \frac{1}{2}\left(\frac{\alpha_k}{\beta_q} + \frac{\beta_q}{\alpha_k}\right)\Lambda_{kq}\,, \qquad v_{kq} = \frac{1}{2}\left(\frac{\alpha_k}{\beta_q} + \frac{\beta_q}{\alpha_k}\right)\Lambda_{kq}\,, \qquad \sum_q \Lambda_{kq}\Lambda_{k'q} = \delta_{kk'} \tag{5.3}$$

with $\alpha_k \in \mathbb{R}$ and $\beta_q \in \mathbb{R}$. Direct insertion shows that the bosonic commutation relations are automatically preserved under such a Bogoliubov transform.

In the general case, interpreting the coefficients as matrix elements $u_{kq} = (U)_{kq}$ and $v_{kq} = (V)_{kq}$ as elements of matrices, we can also write these relations as

$$UU^\dagger - VV^\dagger = \mathbf{1}\,, \qquad UV^{\mathrm{T}} - VU^{\mathrm{T}} = \mathbf{0}\,. \tag{5.4}$$

Now, arranging the U and V matrices in an enlarged matrix

$$W = \begin{pmatrix} U^{\mathrm{T}} & V^\dagger \\ V^{\mathrm{T}} & U^\dagger \end{pmatrix}\,, \qquad W^{\mathrm{T}} = \begin{pmatrix} U & V \\ V^* & U^* \end{pmatrix}\,, \tag{5.5}$$

where A^{T} denotes the transpose of the matrix A, we see that we can encode the conditions (5.4) – or conjugate (transposes) thereof – into a single relation on the matrix W

$$W^{\mathrm{T}} \begin{pmatrix} \mathbf{0} & +\mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix} W = \begin{pmatrix} \mathbf{0} & +\mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix}\,. \tag{5.6}$$

Such matrices W are called **symplectic**, they have unit determinant and form a group under matrix multiplication. Consequently, in general Bogoliubov transforms are symplectic transforms of the creation and annihilation operators. Fortunately, even in the non-trivial cases, the symplectic transform is not completely fixed, which gives us the freedom to recast the Hamiltonian into a specific form.

Formally vectorizing the creation and annihilation operators, the Bogoliubov transform can then be written as

$$\left(\begin{array}{c} \vdots \\ a_k \\ \vdots \\ \hline \vdots \\ a_k^\dagger \\ \vdots \end{array}\right) = \left(\begin{array}{c|c} U & V \\ \hline V^* & U^* \end{array}\right) \left(\begin{array}{c} \vdots \\ b_k \\ \vdots \\ \hline \vdots \\ b_k^\dagger \\ \vdots \end{array}\right) = W^{\mathrm{T}} \left(\begin{array}{c} \vdots \\ b_k \\ \vdots \\ \hline \vdots \\ b_k^\dagger \\ \vdots \end{array}\right)\,. \tag{5.7}$$

Two-mode example

We consider a bosonic reservoir with just two modes that is coupled via the dimensionless operator $S = S^\dagger$ to some arbitrary system H_S

$$\begin{aligned} H &= H_S + \omega_1 \left[a_1^\dagger + \frac{\lambda_1}{\omega_1} S\right]\left[a_1 + \frac{\lambda_1}{\omega_1} S\right] + \omega_2 \left[a_2^\dagger + \frac{\lambda_2}{\omega_2} S\right]\left[a_2 + \frac{\lambda_2}{\omega_2} S\right] \\ &= H_S + \left(\frac{\lambda_1^2}{\omega_1} + \frac{\lambda_2^2}{\omega_2}\right) S^2 + S[\lambda_1(a_1 + a_1^\dagger) + \lambda_2(a_2 + a_2^\dagger)] + \omega_1 a_1^\dagger a_1 + \omega_2 a_2^\dagger a_2 \,. \end{aligned} \tag{5.8}$$

This Hamiltonian has a lower bound for all values of the couplings λ_i, provided that $\omega_i > 0$ and H_S has a lower bound. If $H_S = \omega a^\dagger a$ and $S = \alpha a + \alpha^* a^\dagger$ were bosonic and the full Hamiltonian H was at most quadratic, one could use a general three-mode Bogoliubov transform to write it as a sum of non-interacting modes $H = \Omega_0 c_0^\dagger c_0 + \Omega_1 c_1^\dagger c_1 + \Omega_2 c_2^\dagger c_2$. However, we want to generalize later-on to infinite-size systems, where this approach cannot be applied and, additionally, H_S need not be a bosonic operator in general.

We therefore use the two-mode **Bogoliubov transform**

$$\begin{aligned} a_1 = {} & \frac{1}{2}\left(\frac{\alpha_1}{\beta_1} + \frac{\beta_1}{\alpha_1}\right)\Lambda_{11} b_1 + \frac{1}{2}\left(\frac{\alpha_1}{\beta_2} + \frac{\beta_2}{\alpha_1}\right)\Lambda_{12} b_2 \\ & + \frac{1}{2}\left(\frac{\alpha_1}{\beta_1} - \frac{\beta_1}{\alpha_1}\right)\Lambda_{11} b_1^\dagger + \frac{1}{2}\left(\frac{\alpha_1}{\beta_2} - \frac{\beta_2}{\alpha_1}\right)\Lambda_{12} b_2^\dagger \,, \\ a_2 = {} & \frac{1}{2}\left(\frac{\alpha_2}{\beta_1} + \frac{\beta_1}{\alpha_2}\right)\Lambda_{21} b_1 + \frac{1}{2}\left(\frac{\alpha_2}{\beta_2} + \frac{\beta_2}{\alpha_2}\right)\Lambda_{22} b_2 \\ & + \frac{1}{2}\left(\frac{\alpha_2}{\beta_1} - \frac{\beta_1}{\alpha_2}\right)\Lambda_{21} b_1^\dagger + \frac{1}{2}\left(\frac{\alpha_2}{\beta_2} - \frac{\beta_2}{\alpha_2}\right)\Lambda_{22} b_2^\dagger \,, \end{aligned} \tag{5.9}$$

and likewise for the creation operators. By construction, this transform preserves the bosonic commutation relations. The unknown parameters hidden in the orthogonal matrix Λ_{kq} can be fixed by demanding that the Hamiltonian after the transformation does not include couplings between H_S and the second transformed mode. In particular, with

$$\Lambda = \begin{pmatrix} \lambda_1\alpha_1 & -\lambda_2\alpha_2 \\ +\lambda_2\alpha_2 & \lambda_1\alpha_1 \end{pmatrix} \frac{1}{\sqrt{\lambda_1^2\alpha_1^2 + \lambda_2^2\alpha_2^2}} \tag{5.10}$$

we see that

$$\lambda_1(a_1 + a_1^\dagger) + \lambda_2(a_2 + a_2^\dagger) = \frac{\sqrt{\lambda_1^2\alpha_1^2 + \lambda_2^2\alpha_2^2}}{\beta_1}(b_1 + b_1^\dagger) \,, \tag{5.11}$$

such that the coupling is now only between H_S and the first transformed mode. However, this does not decouple the second transformed mode, since by inserting the same transformation into the term $\omega_1 a_1^\dagger a_1 + \omega_2 a_2^\dagger a_2$, we will automatically generate an interaction between the modes: Since the transformation is linear, the resulting operator will again be at most quadratic between the annihilation and creation operators. In principle, this may also generate terms like b_1^2 and b_2^2, but we still have the freedom to choose the α_i and β_i to prevent the generation of such terms.

- For example, by choosing $\alpha_i = \beta_i = 1$, the Bogoliubov transform becomes a unitary transform that does not mix between creation and annihilation operators, which allows to write

$$\omega_1 a_1^\dagger a_1 + \omega_2 a_2^\dagger a_2 = E_0 + \Omega_1 b_1^\dagger b_1 + \Omega_2 b_2^\dagger b_2 + \Lambda_2 \left(b_1^\dagger b_2 + b_2^\dagger b_1\right) \,, \tag{5.12}$$

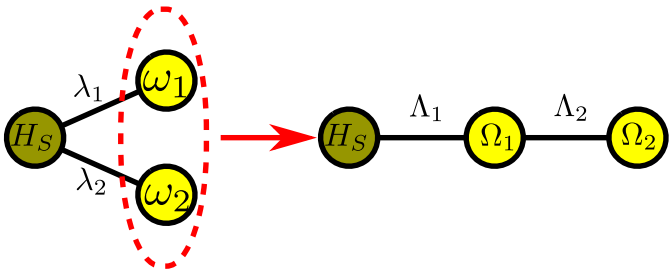

Figure 5.1: Effect of the two-mode Bogoliubov transform. The system (orange) coupled initially to two a modes via couplings λ_1 and λ_2 is after the transformation coupled only to the b_1 mode via Λ_1, which is then coupled to the b_2 mode via Λ_2. Strong-coupling effects can be treated by treating H_S and the b_1 mode explicitly.

where the new frequencies Ω_i and the residual coupling Λ_2 are functions of the λ_i and ω_i, see Fig. 5.1. Interestingly, after the mapping the residual interaction between modes b_1 and b_2 preserves the quasiparticle number. Since we can identify

$$\Lambda_1 = \sqrt{\lambda_1^2\alpha_1^2 + \lambda_2^2\alpha_2^2}/\beta_1\,, \tag{5.13}$$

we see that in the strong-coupling limit $\lambda_i \to \infty$, the system-reaction coordinate coupling will also diverge $\Lambda_1 \to \infty$. However, the matrix elements of the orthogonal matrix Λ will remain finite also in this limit, since its entries are normalized. Therefore, the residual coupling Λ_2 will remain finite.

- Other choices of α_i and β_i lead to decompositions of the form

$$\omega_1 a_1^\dagger a_1 + \omega_2 a_2^\dagger a_2 = E_0 + \Omega_1 b_1^\dagger b_1 + \Omega_2 b_2^\dagger b_2 + \Lambda_2(b_1 + b_1^\dagger)(b_2 + b_2^\dagger)\,, \tag{5.14}$$

which leads to the same situation as in Fig. 5.1, but various combinations may be used. In any case, the coupling Λ_2 need not diverge as $\lambda_i \to \infty$, as the transformation needs to respect the bosonic commutation relations.

If more modes are involved, the transformations become larger, such that to find the suitable mapping transform, larger algebraic problems have to be solved. In particular, for an infinite size reservoir, one will have to resort to other means of finding the suitable transformation.

Derivation of the mapping

We postulate the equivalence of the following Hamiltonians. First, we have

$$\begin{aligned} H &= H_S + \sum_k \omega_k \left(a_k^\dagger + \frac{t_k}{\omega_k} S\right)\left(a_k + \frac{t_k}{\omega_k} S\right) \\ &= \left(H_S + \sum_k \frac{t_k^2}{\omega_k} S^2\right) + S\sum_k t_k\left(a_k + a_k^\dagger\right) + \sum_k \omega_k a_k^\dagger a_k\,, \end{aligned} \tag{5.15}$$

where $H_S = H_S^\dagger$ is an arbitrary system Hamiltonian with a lower spectral bound and $S = S^\dagger$ is an arbitrary dimensionless system operator that couples the system to a bath of harmonic oscillators with spontaneous emission/absorbtion amplitudes t_k and energies ω_k. Note that we have absorbed any phase in the bosonic operators and thereby assume $t_k \in \mathbb{R}$. These amplitudes enter the original **spectral function** as before

$$J^{(0)}(\omega) = 2\pi \sum_k |t_k|^2 \delta(\omega - \omega_k)\,. \tag{5.16}$$

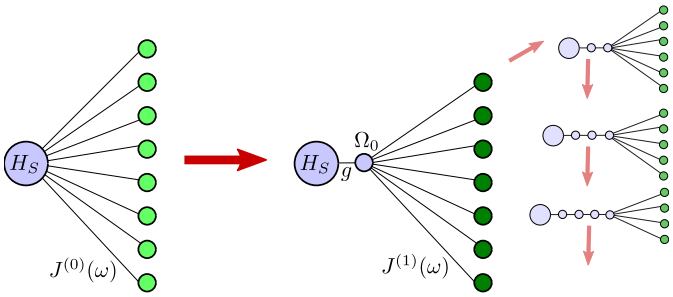

Figure 5.2: Sketch of the reaction-coordinate mapping. The original star-shaped interaction is transformed into a setup where the system couples to the reaction-coordinate, which then couples to all the modes of the residual reservoir. The magnitude of $J^{(0)}(\omega)$ only maps to the magnitude of g, such that arbitrarily strong couplings can be treated, provided $J^{(1)}(\omega)$ admits a perturbative treatment. Recursive application of the mapping leads to a chain representation of the reservoir.

Obviously, the Hamiltonian also has a lower spectral bound.

Second, we say that (up to a possible shift)

$$\begin{aligned} H &= H_S + \Omega_0 \left(b^\dagger + \frac{g}{\Omega_0} S\right)\left(b + \frac{g}{\Omega_0} S\right) + \sum_k \Omega_k \left(b_k^\dagger + \frac{h_k}{\Omega_k}\left(b + b^\dagger\right)\right)\left(b_k + \frac{h_k}{\Omega_k}\left(b + b^\dagger\right)\right) \\ &= H_S + \Omega_0 b^\dagger b + gS(b + b^\dagger) + \frac{g^2}{\Omega_0} S^2 + \sum_k \frac{h_k^2}{\Omega_k}(b + b^\dagger)^2 + (b + b^\dagger)\sum_k h_k \left(b_k + b_k^\dagger\right) + \sum_k \Omega_k b_k^\dagger b_k \,, \end{aligned} \tag{5.17}$$

where b denotes a **reaction coordinate** (RC) and the b_k **residual reservoir** modes. The reaction coordinate has energy Ω_0 and is coupled to the original system via the coupling constant g. The coupling between the reaction coordinate and the residual reservoir is described by the h_k amplitudes, and treating these perturbatively it is useful to define the residual **spectral function** via

$$J^{(1)}(\omega) = 2\pi \sum_k |h_k|^2 \delta(\omega - \Omega_k) \,. \tag{5.18}$$

The intended mapping is visualized in Fig. 5.2.

The mapping shall be achieved by means of a Bogoliubov transform

$$a_k = u_{k0} b + \sum_{q \geq 1} u_{kq} b_q + v_{k0} b^\dagger + \sum_{q \geq 1} v_{kq} b_q^\dagger \tag{5.19}$$

and similar for the creation operator. To maintain the bosonic character of the new modes, the coefficients u_{kq} and v_{kq} have to obey the relations

$$\begin{aligned} 0 &= \sum_q \left(u_{kq} v_{k'q} - v_{kq} u_{k'q}\right) \,, \\ \delta_{kk'} &= \sum_q \left(u_{kq} u_{k'q}^* - v_{kq} v_{k'q}^*\right) \,. \end{aligned} \tag{5.20}$$

This is automatically obeyed when we choose them via

$$u_{kq} = \frac{1}{2}\left(\sqrt{\frac{\omega_k}{\Omega_q}} + \sqrt{\frac{\Omega_q}{\omega_k}}\right)\Lambda_{kq} \,, \qquad v_{kq} = \frac{1}{2}\left(\sqrt{\frac{\omega_k}{\Omega_q}} - \sqrt{\frac{\Omega_q}{\omega_k}}\right)\Lambda_{kq} \,, \tag{5.21}$$

with the unknown orthogonality transformation Λ obeying

$$\sum_q \Lambda_{kq}\Lambda_{k'q} = \delta_{kk'}\,. \tag{5.22}$$

Here, $q = 0$ maps to the annihilation and creation operators of the RC.

Energy and coupling strength of the RC Inserting the transformation and comparing the terms linear in S yields that the first column of the orthogonal transformation has to be chosen as $\Lambda_{k0} = \frac{t_k}{g}\sqrt{\frac{\omega_k}{\Omega_0}}$ and the other ones just orthogonal. Since every row of the orthogonal transformation needs to be normalized $\sum_k \Lambda_{k0}^2 = 1$, we readily obtain the coupling strength to the RC

$$1 = \frac{1}{2\pi g^2\Omega_0}\int_0^\infty \omega J^{(0)}(\omega)d\omega\,. \tag{5.23}$$

Comparing the terms quadratic in S yields the relation

$$\frac{g^2}{\Omega_0} = \frac{1}{2\pi}\int_0^\infty \frac{J^{(0)}(\omega)}{\omega}d\omega\,. \tag{5.24}$$

Furthermore, the terms with $b^\dagger b$ yield

$$\Omega_0 = \frac{1}{2\pi g^2}\int_0^\infty \omega J^{(0)}(\omega)d\omega\,. \tag{5.25}$$

The first and the last of these equations are just the same, and combining the first and the second we can deduce **energy and coupling strength of the RC**

$$\Omega_0^2 = \frac{\int_0^\infty \omega J^{(0)}(\omega)d\omega}{\int_0^\infty \frac{J^{(0)}(\omega)}{\omega}d\omega}\,, \qquad g^2 = \frac{1}{2\pi\Omega_0}\int_0^\infty \omega J^{(0)}(\omega)d\omega\,. \tag{5.26}$$

This is slightly different from the mapping that arises without a manifest lower spectral bound [1]. We remark that $J^{(0)}(\omega)$, Λ, and g all have dimensions of energy. Furthermore, by comparing the terms with $(b + b^\dagger)^2$ we already get a relation between original and transformed spectral densities

$$\frac{4g^2}{2\pi}\int \frac{J^{(1)}(\omega)}{\omega}d\omega = \frac{1}{2\pi\Omega_0^2}\int_0^\infty \omega^3 J^{(0)}(\omega)d\omega - \frac{1}{2\pi}\int_0^\infty \omega J^{(0)}(\omega)d\omega\,, \tag{5.27}$$

which however is unfortunately not explicit.

Mapping of the spectral function We first consider the Heisenberg equations of motion for an arbitrary system observable $\boldsymbol{A} = e^{+\mathrm{i}Ht}Ae^{-\mathrm{i}Ht}$, which become $\dot{\boldsymbol{A}} = e^{+\mathrm{i}Ht}[H, A_S]e^{-\mathrm{i}Ht}$, in the original picture, i.e., based on Eq. (5.15). Specifically, we get (bold symbols denote the Heisenberg picture)

$$\begin{aligned}
\dot{\boldsymbol{A}} &= \mathrm{i}\boldsymbol{S_1} + \mathrm{i}\boldsymbol{S_2}\sum_k t_k(\boldsymbol{a_k} + \boldsymbol{a_k^\dagger})\,,\\
\dot{\boldsymbol{a_k}} &= -\mathrm{i}\omega_k\boldsymbol{a_k} - \mathrm{i}t_k\boldsymbol{S}\,,\\
\dot{\boldsymbol{a_k}}^\dagger &= +\mathrm{i}\omega_k\boldsymbol{a_k^\dagger} + \mathrm{i}t_k\boldsymbol{S}\,,
\end{aligned} \tag{5.28}$$

with

$$\begin{aligned}\boldsymbol{S_1} &= e^{+\mathrm{i}Ht}\left[H_S + \sum_k \frac{t_k^2}{\omega_k} S^2, A\right] e^{-\mathrm{i}Ht}\,,\\ \boldsymbol{S_2} &= e^{+\mathrm{i}Ht}\,[S, A]\, e^{-\mathrm{i}Ht}\,.\end{aligned} \tag{5.29}$$

Next, we perform an FT with the convention that $\Im z \geq 0$

$$A(z) = \int \boldsymbol{A} e^{+\mathrm{i}zt} dt\,. \tag{5.30}$$

This will convert the equations into algebraic ones – we use an overbar do denote the transformed creation operator and use the convolution theorem

$$\begin{aligned}\mathrm{i}zA(z) &= \mathrm{i}S_1(z) + \frac{\mathrm{i}}{2\pi}\int dz' S_2(z') \sum_k t_k \left[a_k(z-z') + \bar{c}_k(z-z')\right]\,,\\ \mathrm{i}z a_k(z) &= -\mathrm{i}\omega_k a_k(z) - \mathrm{i}t_k S(z)\,,\\ \mathrm{i}z \bar{c}_k(z) &= +\mathrm{i}\omega_k \bar{c}_k(z) + \mathrm{i}t_k S(z)\,,\end{aligned} \tag{5.31}$$

of which we can eliminate the last two and insert it in the first, yielding

$$zA(z) = S_1(z) + \frac{1}{2\pi}\int dz' S_2(z') \sum_k t_k^2 \left[\frac{1}{z-z'-\omega_k} - \frac{1}{z-z'+\omega_k}\right] S(z-z') \tag{5.32}$$

Now, we do the same as before, but in the transformed picture based on (5.17), where the Heisenberg equations become

$$\begin{aligned}\dot{\boldsymbol{A}} &= \mathrm{i}\boldsymbol{S_1} + \mathrm{i}\boldsymbol{S_2} g(\boldsymbol{b} + \boldsymbol{b}^\dagger)\,,\\ \dot{\boldsymbol{b}} &= -\mathrm{i}\Omega_0 \boldsymbol{b} - \mathrm{i}g\boldsymbol{S} - 2\mathrm{i}\sum_k \frac{h_k^2}{\Omega_k}(\boldsymbol{b} + \boldsymbol{b}^\dagger) - \mathrm{i}\sum_k h_k(\boldsymbol{b_k} + \boldsymbol{b_k^\dagger})\,,\\ \dot{\boldsymbol{b}}^\dagger &= +\mathrm{i}\Omega_0 \boldsymbol{b}^\dagger + \mathrm{i}g\boldsymbol{S} + 2\mathrm{i}\sum_k \frac{h_k^2}{\Omega_k}(\boldsymbol{b} + \boldsymbol{b}^\dagger) + \mathrm{i}\sum_k h_k(\boldsymbol{b_k} + \boldsymbol{b_k^\dagger})\,,\\ \dot{\boldsymbol{b}}_{\boldsymbol{k}} &= -\mathrm{i}h_k(\boldsymbol{b} + \boldsymbol{b}^\dagger) - \mathrm{i}\Omega_k \boldsymbol{b_k}\,,\\ \dot{\boldsymbol{b}}_{\boldsymbol{k}}^\dagger &= +\mathrm{i}h_k(\boldsymbol{b} + \boldsymbol{b}^\dagger) + \mathrm{i}\Omega_k \boldsymbol{b_k^\dagger}\,.\end{aligned} \tag{5.33}$$

We proceed as before: We Fourier-transform all equations

$$\begin{aligned}zA(z) &= S_1(z) + \frac{1}{2\pi}\int S_2(z') g[b(z-z') + \bar{b}(z-z')])dz'\,,\\ zb(z) &= -\Omega_0 b(z) - gS(z) - 2\sum_k \frac{h_k^2}{\Omega_k}[b(z) + \bar{b}(z)] - \sum_k h_k[b_k(z) + \bar{b}_k(z)]\,,\\ z\bar{b}(z) &= +\Omega_0 \bar{b}(z) + gS(z) + 2\sum_k \frac{h_k^2}{\Omega_k}[b(z) + \bar{b}(z)] + \sum_k h_k[b_k(z) + \bar{b}_k(z)]\,,\\ zb_k(z) &= -h_k[b(z) + \bar{b}(z)] - \Omega_k b_k(z)\,,\\ z\bar{b}_k(z) &= +h_k[b(z) + \bar{b}(z)] + \Omega_k \bar{b}_k(z)\,,\end{aligned} \tag{5.34}$$

then eliminate

$$b_k(z) = \frac{-h_k}{z+\Omega_k}[b(z)+\bar{b}(z)]\,, \qquad \bar{b}_k(z) = \frac{+h_k}{z-\Omega_k}[b(z)+\bar{b}(z)]\,, \tag{5.35}$$

and then successively $\bar{b}(z) - b(z)$, yielding an equation for $\bar{b}(z) + b(z)$

$$\left[\frac{z^2}{\Omega_0} - \Omega_0 - 4\sum_k \frac{h_k^2}{\Omega_k} - 4\sum_k \frac{h_k^2\Omega_k}{z^2-\Omega_k^2}\right][b(z)+\bar{b}(z)] = 2gS(z)\,. \tag{5.36}$$

Inserting this in the first equation yields

$$\begin{aligned} zA(z) &= S_1(z) + \frac{g}{2\pi}\int S_2(z')[b(z-z')+\bar{b}(z-z')]dz' \\ &= S_1(z) + \frac{2g^2}{2\pi}\int S_2(z')\left[\frac{1}{\frac{(z-z')^2}{\Omega_0} - \Omega_0 - 4\sum_k \frac{h_k^2}{\Omega_k} - 4\sum_k \frac{h_k^2\Omega_k}{(z-z')^2-\Omega_k^2}}\right] S(z-z')dz'\,. \end{aligned} \tag{5.37}$$

Finally, we can compare Eq. (5.32) and Eq. (5.37), which yields a relation between the spectral densities

$$\sum_k t_k^2\left[\frac{1}{z-z'-\omega_k} - \frac{1}{z-z'+\omega_k}\right] = \frac{2g^2}{\frac{(z-z')^2}{\Omega_0} - \Omega_0 - 4\sum_k \frac{h_k^2}{\Omega_k} - 4\sum_k \frac{h_k^2\Omega_k}{(z-z')^2-\Omega_k^2}}\,. \tag{5.38}$$

Going to the continuum limit then implies

$$\frac{1}{\pi}\int_0^\infty \frac{J^{(0)}(\omega)\omega}{(z-z')^2-\omega^2}d\omega = \frac{2g^2}{\frac{(z-z')^2}{\Omega_0} - \Omega_0 - \frac{4}{2\pi}\int_0^\infty \frac{J^{(1)}(\omega)}{\omega}d\omega - \frac{4}{2\pi}\int_0^\infty \frac{J^{(1)}(\omega)\omega}{(z-z')^2-\omega^2}d\omega}\,. \tag{5.39}$$

Introducing the **Cauchy transform of an odd function** $J(\omega)$ via

$$W(z) = \frac{2}{\pi}\int_0^\infty \frac{\omega J(\omega)}{\omega^2-z^2}d\omega = \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{J(\omega')}{\omega'-z}d\omega'\,, \tag{5.40}$$

we see that it has the appealing property

$$\begin{aligned} W(\omega+\mathrm{i}0^+) &= \lim_{\epsilon\to 0^+}\frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{J(\omega')d\omega'}{\omega'-\omega-\mathrm{i}\epsilon} = \lim_{\epsilon\to 0^+}\frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{J(\omega')\left[\omega'-\omega+\mathrm{i}\epsilon\right]}{(\omega'-\omega)^2+\epsilon^2}d\omega' \\ &= \frac{1}{\pi}\mathcal{P}\int\frac{J(\omega')}{\omega'-\omega}d\omega' + \mathrm{i}J(\omega)\,, \end{aligned} \tag{5.41}$$

where we have used a representation of the Dirac-Delta function and $\mathcal{P}$ denotes the Cauchy principal value. Computing the Cauchy transform of both spectral functions we can write Eq. (5.39) as

$$-\frac{1}{2}W^{(0)}(z-z') = \frac{2g^2}{\frac{(z-z')^2}{\Omega_0} - \Omega_0 - \frac{2}{\pi}\int_0^\infty \frac{J^{(1)}(\omega)}{\omega}d\omega + W^{(1)}(z-z')} \tag{5.42}$$

Rearranging this for $W^{(1)}(z-z')$ and evaluating at $z-z'=\omega+\mathrm{i}0^+$ eventually yields the sought-after relation between the spectral functions

$$J^{(1)}(\omega)=\frac{4g^2J^{(0)}(\omega)}{\left[\frac{1}{\pi}\mathcal{P}\int\frac{J^{(0)}(\omega')}{\omega-\omega'}d\omega'\right]^2+\left[J^{(0)}(\omega)\right]^2}\,. \tag{5.43}$$

To summarize, the mapping between Hamiltonians (5.15) and (5.17) is realized by the **phonon mapping**.

Def. 2 (phonon mapping)**.** *The phonon-form of the reaction coordinate mapping for Hamiltonians with lower spectral bound is realized by the transformations for reaction coordinate energy Ω_0, coupling strength g, and residual spectral function $J^{(1)}(\omega)$, that are fully defined by the original spectral function*

$$\begin{aligned}\Omega_0^2&=\frac{\int_0^\infty\omega J^{(0)}(\omega)d\omega}{\int_0^\infty\frac{J^{(0)}(\omega)}{\omega}d\omega}\,,\qquad g^2=\frac{1}{2\pi\Omega_0}\int_0^\infty\omega J^{(0)}(\omega)d\omega\,,\\ J^{(1)}(\omega)&=\frac{4g^2J^{(0)}(\omega)}{\left[\frac{1}{\pi}\mathcal{P}\int\frac{J^{(0)}(\omega')}{\omega-\omega'}d\omega'\right]^2+\left[J^{(0)}(\omega)\right]^2}\,,\end{aligned} \tag{5.44}$$

where the analytic continuation $J^{(0)}(-\omega)=-J^{(0)}(\omega)$ is understood.

- The first observation is that if we rescale the original spectral function by a factor α, g^2 will scale proportional to α as well, such that this factor α will cancel in the numerator and denominator. Thereby, the ultrastrong coupling limit in the original frame $\alpha\to\infty$ will have absolutely no effect on the coupling strength to the residual reservoir. Rather, the coupling strength to the residual reservoir will depend on the shape of the original spectral function.

- By redefining $S=(b+b^\dagger)$ in Eq. (5.17) and absorbing the reaction coordinate terms into H_S, we see that the form of (5.15) is fully reproduced, such that the mapping transformation can be iterated recursively, until one of the involved integrals diverges. For the recursive application, the above definition can be used with simply replacing $J^{(0)}(\omega)\to J^{(n)}(\omega)$ and $J^{(1)}(\omega)\to J^{(n+1)}(\omega)$.

- Finally, for spectral functions that have a finite support, i.e., which are non-vanishing only inside a region $\omega\in[0,\omega_m]$, one can show that the mapping transformations lead to the limiting spectral function [2]

$$\bar{J}(\omega)=\omega\sqrt{1-\frac{\omega^2}{\omega_m^2}}\Theta(\omega_m^2-\omega^2)\,, \tag{5.45}$$

  known as **Rubin spectral function**. Direct insertion into the mapping relation shows that it reproduces itself under the mapping. The observation that it has a maximum at $\omega_m/\sqrt{2}$ of height $\omega_m/2$ shows that for large ω_m, the limiting spectral function need not be small. In such cases, it is better to split the initial spectral function into intervals of small width ω_m and then apply such mappings to each interval individually.

Benchmark: Spin-boson model

We consider a single-reservoir scenario with

$$H = \frac{\omega}{2}\sigma^z + \sum_k \frac{t_k^2}{\omega_k} S^2 + S\sum_k t_k \left(a_k + a_k^\dagger\right) + \sum_k \omega_k a_k^\dagger a_k \,, \tag{5.46}$$

where $S = \sigma^z$ can implement either the exactly solvable pure-dephasing limit and $S = \sigma^x$ would be a dissipative spin-boson model. Since in these cases $S^2 = \mathbf{1}$, the renormalization term corresponds to a trivial shift. To compare with an available exact solution, we will consider the pure-dephasing limit $S = \sigma^z$ here, but the method is applicable more generally. As an example, the original spectral function shall be

$$J^{(0)}(\omega) = 2\pi \sum_k |t_k|^2 \delta(\omega - \omega_k) = \Gamma \frac{\omega\delta^7}{\left[(\omega-\epsilon)^2+\delta^2\right]^2\left[(\omega+\epsilon)^2+\delta^2\right]^2} \,, \tag{5.47}$$

where Γ denotes an overall coupling strength, and for $\epsilon > \delta > 0$ the parameter ϵ describes roughly the position of the maximum and δ roughly the width around the maximum. All these parameters have dimension of energy. This special spectral function is chosen to perform the mapping analytically.

Accordingly, the transformed model reads

$$H = \frac{\omega}{2}\sigma^z + \Omega_0 \left(b^\dagger + \frac{g}{\Omega_0}S\right)\left(b + \frac{g}{\Omega_0}S\right) + \sum_k \Omega_k \left(b_k^\dagger + \frac{h_k}{\Omega_k}(b+b^\dagger)\right)\left(b_k + \frac{h_k}{\Omega_k}(b+b^\dagger)\right) \,, \tag{5.48}$$

where the energy of the RC and the coupling strength become

$$\Omega_0^2 = \frac{\left(\delta^2+\epsilon^2\right)^2}{5\delta^2+\epsilon^2} \,, \qquad g^2 = \frac{\Gamma\delta^4\sqrt{5\delta^2+\epsilon^2}}{64\left(\delta^2+\epsilon^2\right)^2} \,. \tag{5.49}$$

The mapping transformation can be computed explicitly, where the transformed spectral function becomes ohmic

$$J^{(1)}(\omega) = \frac{16\omega\delta^3\sqrt{5\delta^2+\epsilon^2}}{\omega^4 + \omega^2(6\delta^2 - 2\epsilon^2) + (5\delta^2+\epsilon^2)^2} \,, \tag{5.50}$$

which does not depend on the coupling strength Γ (demonstrating that it can be chosen arbitrarily large). With introducing the supersystem renormalization (for the chosen spectral function, everything converges)

$$\Omega_0 \cdot \Delta \equiv \sum_k \frac{h_k^2}{\Omega_k} = \frac{1}{2\pi}\int_0^\infty \frac{J^{(1)}(\omega)}{\omega} d\omega \,, \tag{5.51}$$

we can identify a new decomposition into supersystem H'_S and residual reservoir H'_B via $H = H'_S + H'_B + H'_I$ with

$$\begin{aligned} H'_S &= \frac{\omega}{2}\sigma^z + \Omega_0\left(b^\dagger + \frac{g}{\Omega_0}S\right)\left(b + \frac{g}{\Omega_0}S\right) + \Omega_0\Delta(b+b^\dagger)^2 \,, \\ H'_I &= (b+b^\dagger)\sum_k h_k(b_k + b_k^\dagger) \,, \qquad H'_B = \sum_k \Omega_k b_k^\dagger b_k \,, \end{aligned} \tag{5.52}$$

for which we can derive and solve a master equation in the usual way. For the sake of simplicity we will not bother to derive a Lindblad master equation but will simply use the Redfield master equation, but now for the supersystem

$$\dot{\rho} = -\mathrm{i}\left[H'_S, \rho\right] - \int_0^\infty C(+\tau)\left[(b+b^\dagger), e^{-\mathrm{i}H'_S\tau}(b+b^\dagger)e^{+\mathrm{i}H'_S\tau}\rho(t)\right]d\tau \\ - \int_0^\infty C(-\tau)\left[\rho(t)e^{-\mathrm{i}H'_S\tau}(b+b^\dagger)e^{+\mathrm{i}H'_S\tau}, (b+b^\dagger)\right]d\tau\,. \tag{5.53}$$

Here, $C(\tau)$ is the correlation function for the residual bath

$$C(\tau) = \frac{1}{2\pi}\int \gamma(\omega)e^{-\mathrm{i}\omega\tau}d\omega = \frac{1}{2\pi}\int J^{(1)}(\omega)[1+n_B(\omega)]e^{-\mathrm{i}\omega\tau}d\omega\,, \tag{5.54}$$

which under the assumption of weak residual coupling (for which we have derived the master equation) is still approximately in a thermal state with the same temperature. The half-sided Fourier transform can be performed by finding the eigenbasis of the supersystem Hamiltonian $H'_S\left|a'\right\rangle = E'_a\left|a'\right\rangle$, such that

$$\int_0^\infty C(\tau)e^{-\mathrm{i}H'_S\tau}(b+b^\dagger)e^{+\mathrm{i}H'_S\tau}d\tau = \sum_{ab}\left\langle a'\right|(b+b^\dagger)\left|b'\right\rangle\int_0^\infty C(\tau)e^{-\mathrm{i}(E'_a-E'_b)\tau}d\tau\left|a'\right\rangle\left\langle b'\right|\,. \tag{5.55}$$

Now, the remaining half-sided integral can be evaluated via

$$\int_0^\infty C(\tau)e^{+\mathrm{i}(E'_b-E'_a)\tau}d\tau = \int\Theta(\tau)C(\tau)e^{+\mathrm{i}(E'_b-E'_a)\tau}d\tau = \int d\omega\gamma(\omega)\left[\frac{1}{2\pi}\int d\tau e^{+\mathrm{i}(E'_b-E'_a-\omega)\tau}\frac{1}{2}[1+\mathrm{sgn}(\tau)]\right] \\ = \frac{\gamma(E'_b-E'_a)}{2} + \frac{\mathrm{i}}{2\pi}\mathcal{P}\int\frac{\gamma(\omega)}{E'_b-E'_a-\omega}d\omega \approx \frac{\gamma(E'_b-E'_a)}{2} \tag{5.56}$$

where in the last equality sign we have neglected the Lamb shift. The dissipator can then be established numerically, after obtaining the eigenbasis of H'_S.

The solution for the supersystem $\rho(t)$ then allows to compute observables such as the absolute value of coherences

$$|\rho_{01}| = \left|\frac{1}{2}\mathrm{Tr}\left\{(\sigma^x+\mathrm{i}\sigma^y)\rho(t)\right\}\right|, \tag{5.57}$$

which can be directly compared with the exact solution that we derived previously. Likewise, we had established that due to global energy conservation, the energy radiated into the reservoir must stem from the interaction

$$\frac{d}{dt}\left\langle\sum_k\omega_k a_k^\dagger a_k\right\rangle = -\frac{d}{dt}\left\langle\sigma^z\sum_k t_k(a_k+a_k^\dagger)\right\rangle = -\frac{d}{dt}g\left\langle\sigma^z(b+b^\dagger)\right\rangle\,, \tag{5.58}$$

where the last expression is now accessible within the master equation formulation of the supersystem and can be compared with the exact solution for the current obtained from the time derivative of of the reservoir energy, provided the supersystem is initialized as

$$\rho_0 = \rho_S^0\otimes\frac{e^{-\beta\Omega\left[b^\dagger b+\Delta(b+b^\dagger)^2\right]}}{Z_{RC}}\,, \tag{5.59}$$

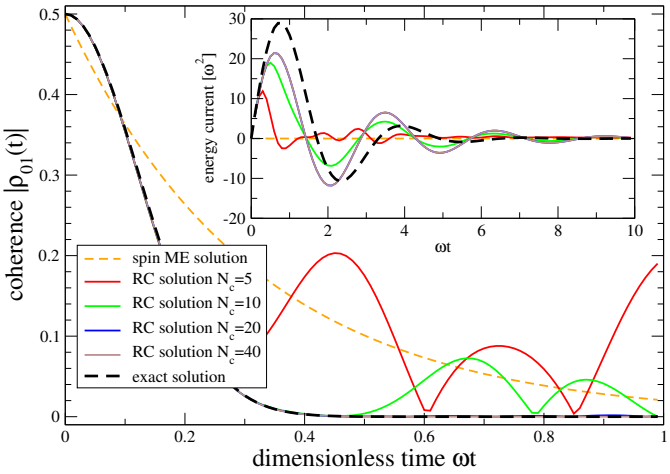

Figure 5.3: Evolution of coherences in the pure-dephasing spin boson model and energy radiated into the reservoir versus dimensionless time. Whereas the naive master equation for the single spin predicts simple exponential decay and a vanishing energy current (orange dashed), treatment of the supersystem (solid curves) approximates the exact solution (bold dashed black) much better, depending on the bosonic cutoff chosen. To compute the currents (inset) more accurately, further mappings would be necessary. Parameters: $\Gamma\beta = 10000$, $\delta\beta = 1$, $\epsilon\beta = 2$, $\omega\beta = 1$.

where the first factor is the initial state of the spin (including e.g. coherences) and the second part comes from the reduced thermal state of the reaction coordinate. The result is depicted in Fig. 5.3. One can see that the transient evolution of coherences is extremely well captured with the RC approach. By further increasing the bosonic cutoff N_c, the solution well approaches the exact one. The total radiated current however dows not yet approximate the exact solution well (even for $N_c \to \infty$), which roots in the Markovian approximation applied to the supersystem ($\delta\beta \approx 1$ does not fully justify a Markovian treatment). The bottom-line is that a time-local (and in this sense Markovian) treatment of the supersystem includes non-Markovian effects in the original system.

5.3.2 Fermionic reaction-coordinate mappings

As for bosonic systems, similar Bogoliubov transforms exist for fermionic systems. The only difference is that they preserve the fermionic anticommutation relations.

Fermionic Bogoliubov transforms

Def. 3 (Fermionic Bogoliubov transform)**.** *A fermionic Bogoliubov transform is a linear mapping between fermionic annihilation and creation operators, which preserves the corresponding fermionic anticommutation relations*

$$c_k = \sum_q \left[u_{kq} d_q + v_{kq} d_q^\dagger\right] , \qquad \begin{aligned} \left\{c_k, c_{k'}^\dagger\right\} &= \delta_{kk'} , & \{c_k, c_{k'}\} &= 0 , \\ \left\{d_k, d_{k'}^\dagger\right\} &= \delta_{kk'} , & \{d_k, d_{k'}\} &= 0 , \end{aligned} \tag{5.60}$$

where $u_{kq}, v_{kq} \in \mathbb{C}$.

In analogy to the bosonic case, the constraints that the coefficients u_{kq} and v_{kq} have to obey can be written as

$$\sum_q \left(u_{kq} u_{k'q}^* + v_{kq} v_{k'q}^*\right) = \delta_{kk'} , \qquad \sum_q \left(u_{kq} v_{k'q} + v_{kq} u_{k'q}\right) = 0 , \tag{5.61}$$

or in matrix notation

$$UU^\dagger + VV^\dagger = \mathbf{1}\,, \qquad UV^{\mathrm{T}} + VU^{\mathrm{T}} = \mathbf{0}\,. \tag{5.62}$$

In the following, we will only treat the case of particle-conserving interactions (relevant e.g. for electronic tunneling), such that when we consider just $V = 0$, again U just needs to be a unitary transformation to obey the preservation of the anticommutation relations. Another simplification is that we will not bother to write the Hamiltonian in a manifestly positive form, since for fermions the spectrum is always bounded from below.

Two-mode example

Consider the fermionic Hamiltonian

$$H = H_S + \left(t_1 d^\dagger c_1 + t_1^* c_1^\dagger d\right) + \left(t_2 d^\dagger c_2 + t_2^* c_2^\dagger d\right) + \varepsilon_1 c_1^\dagger c_1 + \varepsilon_2 c_2^\dagger c_2\,, \tag{5.63}$$

where H_S may contain arbitrary interactions and d is an operator in the system. A unitary Bogoliubov transform of the reservoir modes only

$$c_1 = u_{11} d_1 + u_{12} d_2\,, \qquad c_2 = u_{21} d_1 + u_{22} d_2\,, \tag{5.64}$$

and analogous for the creation operators can now be chosen to achieve an effective decoupling of the system and the second mode d_2. Inserting this transformation

$$\begin{aligned} H = H_S &+ \left[d^\dagger(t_1 u_{11} + t_2 u_{21}) d_1 + d^\dagger(t_1 u_{12} + t_2 u_{22}) d_2 + \text{h.c.}\right] \\ &+ \varepsilon_1 \left(u_{11}^* d_1^\dagger + u_{12}^* d_2^\dagger\right)(u_{11} d_1 + u_{12} d_2) + \varepsilon_2 \left(u_{21}^* d_1^\dagger + u_{22}^* d_2^\dagger\right)(u_{21} d_1 + u_{22} d_2)\,, \end{aligned} \tag{5.65}$$

and we see that by fulfilling $(t_1 u_{12} + t_2 u_{22}) = 0$ we can achieve a decoupling of the system and the second mode. This is for example implemented by the choice

$$U = \frac{1}{\sqrt{|t_1|^2 + |t_2|^2}} \begin{pmatrix} +t_1^* & -t_2 \\ +t_2^* & +t_1 \end{pmatrix}\,, \tag{5.66}$$

which eventually yields

$$\begin{aligned} H = H_S &+ \left[\underbrace{\sqrt{|t_1|^2 + |t_2|^2}}_{T_1} d^\dagger d_1 + \text{h.c.}\right] + \underbrace{\frac{\varepsilon_1 |t_1|^2 + \varepsilon_2 |t_2|^2}{|t_1|^2 + |t_2|^2}}_{\epsilon_1} d_1^\dagger d_1 + \underbrace{\frac{\varepsilon_1 |t_2|^2 + \varepsilon_2 |t_1|^2}{|t_1|^2 + |t_2|^2}}_{\epsilon_2} d_2^\dagger d_2 \\ &+ \left[\underbrace{\frac{t_1 t_2}{|t_1|^2 + |t_2|^2}(\varepsilon_2 - \varepsilon_1)}_{T_2} d_1^\dagger d_2 + \text{h.c.}\right]\,, \end{aligned} \tag{5.67}$$

which has the same interpretation as Fig. 5.1 with the appropriately renamed parameters. As before, we see that as $t_i \to \infty$, only T_1 diverges, whereas ϵ_i and also T_2 remain finite. Therefore, an explicit treatment of only the first mode allows for a perturbative treatment also in the strong-coupling limit.

Derivation of the mapping

We postulate the equivalence of the Hamiltonians

$$\begin{aligned} H &= H_S + c\sum_k t_k^* c_k^\dagger - c^\dagger \sum_k t_k c_k + \sum_k \epsilon_k c_k^\dagger c_k \\ &= H_S + \lambda c d^\dagger - \lambda c^\dagger d + \varepsilon d^\dagger d + d\sum_k T_k^* d_k^\dagger - d^\dagger \sum_k T_k d_k + \sum_k \varepsilon_k d_k^\dagger d_k \,. \end{aligned} \tag{5.68}$$

In the first one, t_k gives rise to the original spectral function

$$\Gamma^{(0)}(\omega) = 2\pi \sum_k |t_k|^2 \delta(\omega - \epsilon_k) \,, \tag{5.69}$$

and in the second Hamiltonian, λ and ε denote coupling and energy of the reaction coordinate, respectively. Also, the amplitudes T_k and energies ε_k define the residual spectral function

$$\Gamma^{(1)}(\omega) = 2\pi \sum_k |T_k|^2 \delta(\omega - \varepsilon_k) \,. \tag{5.70}$$

Thus, the difference to the bosonic case is that no extra term is required to grant the existence of a lower bound and also that the spectral functions can be defined also for negative frequencies, such that no analytic continuation is necessary. The transformation shall be implemented by a unitary variant of the Bogoliubov transform

$$c_k = \sum_q u_{kq} d_q \,, \tag{5.71}$$

and specifically we identify $d_0 = d$ as the reaction coordinate.

Energy and coupling strength Thereby, it has to hold that

$$\lambda d = \sum_k t_k c_k \,, \qquad \lambda d^\dagger = \sum_k t_k^* c_k^\dagger \tag{5.72}$$

and similar for the conjugate transpose, such that by computing e.g. the anticommutator of the two terms above we get the relation

$$\lambda^2 = \sum_k |t_k|^2 \,, \tag{5.73}$$

which defines the coupling strength of the reaction coordinate. Solving for d, we get

$$d = \sum_k \frac{t_k}{\lambda} c_k = \sum_k (U^\dagger)_{0k} c_k = \sum_k u_{k0}^* c_k \qquad \Longrightarrow \qquad u_{k0} = \frac{t_k^*}{\lambda} \,. \tag{5.74}$$

Finally, the term that generates the energy of the reaction coordinate must generate from the reservoir Hamiltonian, such that

$$\varepsilon d^\dagger d = \sum_k \epsilon_k |u_{k0}|^2 d^\dagger d = \sum_k \epsilon_k \frac{|t_k|^2}{\lambda^2} d^\dagger d \,. \tag{5.75}$$

This yields the energy of the reaction coordinate

$$\varepsilon = \sum_k \epsilon_k \frac{|t_k|^2}{\lambda^2} \,. \tag{5.76}$$

In the continuum limit, we can get the coupling and energy from integrals over the complete energies

$$\lambda^2 = \frac{1}{2\pi} \int \Gamma^{(0)}(\omega) d\omega \,, \qquad \varepsilon = \frac{1}{2\pi\lambda^2} \int \omega \Gamma^{(0)}(\omega) d\omega \,. \tag{5.77}$$

Mapping of the spectral function To find the mapping relation for the spectral function, we set up the Heisenberg equations of motion for both realizations of the total Hamiltonian. For simplicity, we only consider the Heisenberg equations for the creation and annihilation operators (in principle, any observable can be constructed from these). In the original representation, they become

$$\dot{c} = \mathrm{i}[H_S, c] + \mathrm{i} \sum_k t_k c_k = \mathrm{i} S(t) + \mathrm{i} \sum_k t_k c_k \,, \qquad \dot{c}_k = \mathrm{i} t_k^* c - \mathrm{i} \epsilon_k c_k \,, \tag{5.78}$$

and similarly for the creation operators. Since at this level they do not mix, we consider only the annihilation operators. Fourier-transformation yields

$$z c(z) = S(z) + \sum_k t_k c_k(z) \,, \qquad z c_k(z) = t_k^* c(z) - \epsilon_k c_k(z) \,. \tag{5.79}$$

Eliminating the second equation then gives

$$z c(z) = S_1(z) + \sum_k \frac{|t_k|^2}{z + \epsilon_k} c(z) \,. \tag{5.80}$$

In contrast, the mapped representation yields

$$\dot{c} = \mathrm{i} S(t) + \mathrm{i} \lambda d \,, \qquad \dot{d} = -\mathrm{i}\lambda c - \mathrm{i}\epsilon d + \mathrm{i} \sum_k T_k d_k \,, \qquad \dot{d}_k = \mathrm{i} T_k^* d - \mathrm{i} \epsilon_k d_k \,. \tag{5.81}$$

Fourier-transforming and eliminating the non-system variables then gives

$$z c(z) = S(z) - \frac{\lambda^2}{z + \epsilon - \sum_k \frac{|T_k|^2}{z + \epsilon_k}} c(z) \,, \tag{5.82}$$

and from comparison we get the relation

$$\sum_k \frac{|t_k|^2}{z + \epsilon_k} = - \frac{\lambda^2}{z + \epsilon - \sum_k \frac{|T_k|^2}{z + \epsilon_k}} \,. \tag{5.83}$$

Converting the sums to integrals and evaluating at $z = -\omega + \mathrm{i}\delta$ when $\delta \to 0^+$ we obtain a mapping relation between the fermionic spectral functions just as before.

Summarizing, we obtain the fermionic particle mapping.

Def. 4 (Fermionic particle mapping)**.** *The particle form of the reaction-coordinate mapping for fermionic tunneling Hamiltonians provides the reaction coordinate coupling λ, the energy ε, and the residual spectral function $\Gamma^{(1)}(\omega)$*

$$\lambda^2 = \frac{1}{2\pi}\int \Gamma^{(0)}(\omega)d\omega\,, \qquad \varepsilon = \frac{1}{2\pi\lambda^2}\int \omega\Gamma^{(0)}(\omega)d\omega\,,$$
$$\Gamma^{(1)}(\omega) = \frac{4\lambda^2\Gamma^{(0)}(\omega)}{\left[\frac{1}{\pi}\mathcal{P}\int\frac{\Gamma^{(0)}(\omega')}{\omega-\omega'}d\omega'\right]^2 + [\Gamma^{(0)}(\omega)]^2}\,. \tag{5.84}$$

- As before, the transformed specral density remains invariant under trivial rescalings of the original one.
- As before, the mapping can be performed recursively.
- For spectral functions with a finite support, i.e., nonvanishing ones in the interval $\omega \in [\epsilon-\delta, \epsilon+\delta]$, the mapping converges to a semicircle-shaped spectral density

$$\bar{\Gamma}(\omega) = \delta\sqrt{1-\left(\frac{\omega-\epsilon}{\delta}\right)^2}\,\Theta(\delta^2-(\omega-\epsilon)^2)\,. \tag{5.85}$$

  This has a maximum of δ at $\omega=\epsilon$, which demonstrates that a master equation may just not be applicable for large δ. In such cases, it is better to split the support of the spectral function into small intervals and perform the mapping individually for each interval.

Benchmark: Single-electron transistor

We consider the SET

$$H = \epsilon d^\dagger d + \sum_\nu\sum_k\left[\epsilon_{k\nu}c_{k\nu}^\dagger c_{k\nu} + \left(t_{k\nu}d^\dagger c_{k\nu} + \text{h.c.}\right)\right] \tag{5.86}$$

with two leads $\nu\in\{L,R\}$ described by Lorentzian spectral densities

$$\Gamma_\alpha^{(0)}(\omega) = 2\pi\sum_k |t_{k\nu}|^2\delta(\omega-\epsilon_{k\nu}) = \Gamma_\alpha\frac{\delta_\alpha^2}{(\omega-\epsilon_\alpha)^2+\delta_\alpha^2}\,, \tag{5.87}$$

where $\alpha\in\{L,R\}$ denotes the lead, Γ_α the coupling strength, δ_α the width, and ϵ_α the frequency with the strongest coupling. The wideband limit is implemented with $\delta_\alpha\to\infty$.

Introducing a separate reaction coordinate for each reservoir, the model is transformed into a triple quantum dot (TQD) structure

$$H = H_{TQD} + \sum_\nu\sum_k\left[\varepsilon_{k\nu}d_{k\nu}^\dagger d_{k\nu} + \left(T_{k\nu}d_\nu^\dagger d_{k\nu} + \text{h.c.}\right)\right]\,,$$
$$H_{TQD} = \varepsilon_L d_L^\dagger d_L + \epsilon d^\dagger d + \varepsilon_R d_R^\dagger d_R + \left(\lambda_L d^\dagger d_L + \lambda_R d^\dagger d_R + \text{h.c.}\right)\,, \tag{5.88}$$

where the coupling strengths and energies of the RC, respectively, become

$$\lambda_\nu = \sqrt{\frac{\Gamma_\nu \delta_\nu}{2}}\,, \qquad \varepsilon_\nu = \epsilon_\nu\,. \tag{5.89}$$

Here, for the computation of the RC energy one can actually use symmetry arguments or use the principal value as otherwise the integral is not convergent. The computation of the principal value integral yields

$$\begin{aligned}\mathcal{P}\int \frac{\Gamma_\nu^{(0)}(\omega')}{\omega-\omega'}d\omega' &= 2\pi \mathrm{i}\left[\mathrm{Res}_{\omega'=\epsilon_\nu+\mathrm{i}\delta}\frac{\Gamma_\nu^{(0)}(\omega')}{\omega-\omega'}+\frac{1}{2}\mathrm{Res}_{\omega'=\omega}\frac{\Gamma_\nu^{(0)}(\omega')}{\omega-\omega'}\right]\\ &= \frac{\pi\Gamma_\nu\delta_\nu(\omega-\epsilon_\nu)}{(\omega-\epsilon_\nu)^2+\delta_\nu^2}\,,\end{aligned} \tag{5.90}$$

which eventually allows to compute the residual spectral density

$$\Gamma_\nu^{(1)}(\omega) = 2\pi\sum_k |T_{k\nu}|^2\delta(\omega-\varepsilon_{k\nu}) = 2\delta_\nu\,, \tag{5.91}$$

which is just flat. An additional transformation could not be performed here, since the spectral densities would just diverge. We can now solve the model with various approaches.

- First, since the model is exactly solvable, we can use e.g. nonequilibrium Greens functions or the Laplace transform method (without invoking the wideband limit on the single dot or applying it to the TQD) to obtain an exact solution for the stationary currents in terms of a Landauer representation

$$I_M = \frac{1}{2\pi}\int d\omega T(\omega)[f_L(\omega)-f_R(\omega)]d\omega\,, \tag{5.92}$$

  where the transmission becomes

$$T(\omega) = \frac{\Gamma_L^{(0)}(\omega)\Gamma_R^{(0)}(\omega)}{\left[\omega-\epsilon-\frac{1}{2\pi}\mathcal{P}\int\frac{\Gamma_L^{(0)}(\omega')+\Gamma_R^{(0)}(\omega')}{\omega-\omega'}d\omega'\right]^2+\left[\frac{\Gamma_L^{(0)}(\omega')+\Gamma_R^{(0)}(\omega')}{2}\right]^2}\,. \tag{5.93}$$

- Second, we can use the naive master equation for the SET as discussed explicitly before. From this, we know that the current I_M will scale linarly with the coupling strength if symmetrically coupled $\Gamma_L = \Gamma_R$.

- Third, we can derive the Pauli rate equations for the resulting triple-dot system, which are sometimes referred to as global Lindblad equations, since their Lindblad operators are expressable by the energy eigenbasis of the TQD. Without coherences in the energy eigenbasis, this will correspond to a classical stochastic process switching between the energy eigenstates of the TQD (which can for our example actually be analytically calculated). This master equation is globally of Lindblad form, and therefore the dynamics will be contractive (or Markovian), such that the TQD density matrix will always approach its steady state as enforced by Spohn's inequality. However, the dynamics of the central dot alone does not follow

a master equation and may be non-Markovian. The reduced density matrix of the central dot is always diagonal

$$\rho_c(t) = \begin{pmatrix} 1 - P_1(t) & 0 \\ 0 & P_1(t) \end{pmatrix}, \tag{5.94}$$

and is thereby fully determined by the probability of the central dot being occupied $P_1(t) = \mathrm{Tr}\left\{d^\dagger d\rho(t)\right\}$. Likewise its stationary limit is given by $\bar{P}_1 = \mathrm{Tr}\left\{d^\dagger d\bar{\rho}\right\}$, such that the trace distance between the single-electron density matrix and its stationary limit $T(\rho_c(t), \bar{\rho}_c) = \left|P_1(t) - \bar{P}_1\right|$ or likewise the quantum relative entropy between these states may actually temporarily increase. This hallmarks a non-Markovian effect, demonstrating that the TQD Lindblad equation provides a Markovian embedding for a non-Markovian evolution of the central dot.

- Fourth, we can use the nonsecular Redfield master equation for the triple quantum dot, which is not of Lindblad form but will approximately preserve the density matrix properties when applied within its range of validity (weak residual coupling $\beta_\nu \delta_\nu \ll 1$). In this case, a temporarily increasing trace distance to the stationary state may already be observed in the supersystem.

- Fifth, since the mapping to the triple quantum dot picture does not require the strong-coupling limit, we can also compare with the case where the internal amplitudes λ_ν and the residual amplitudes $T_{k\nu}$ are of the same order by defining the transformation to the interaction picture differently. This results in a **local Lindblad** master equation [3] for the triple quantum dot

$$\begin{aligned}\dot{\rho} = &-\mathrm{i}\left[H_{TQD}, \rho\right] \\ &+ \Gamma_L^{(1)}(\epsilon_L)[1 - f_L(\epsilon_L)]\left[d_L \rho d_L^\dagger - \frac{1}{2}\left\{d_L^\dagger d_L, \rho\right\}\right] + \Gamma_L^{(1)}(\epsilon_L) f_L(\epsilon_L)\left[d_L^\dagger \rho d_L - \frac{1}{2}\left\{d_L d_L^\dagger, \rho\right\}\right] \\ &+ \Gamma_R^{(1)}(\epsilon_R)[1 - f_R(\epsilon_R)]\left[d_R \rho d_R^\dagger - \frac{1}{2}\left\{d_R^\dagger d_R, \rho\right\}\right] + \Gamma_R^{(1)}(\epsilon_R) f_R(\epsilon_R)\left[d_R^\dagger \rho d_R - \frac{1}{2}\left\{d_R d_R^\dagger, \rho\right\}\right],\end{aligned} \tag{5.95}$$

where the coupling between the left and right dots is only mediated by the triple dot Hamiltonian H_{TQD}.

The results of these considerations are shown in Fig. 5.4. One can see that a single Lindblad approach – at least of the forms mentioned – is not able to capture the behaviour of the exact solution for all coupling strengths, whereas the Redfield master equation, despite not obeying the Lindblad form, captures its features much better over a wide range of parameters. Nevertheless, for particular regimes suitable Lindblad descriptions exist.

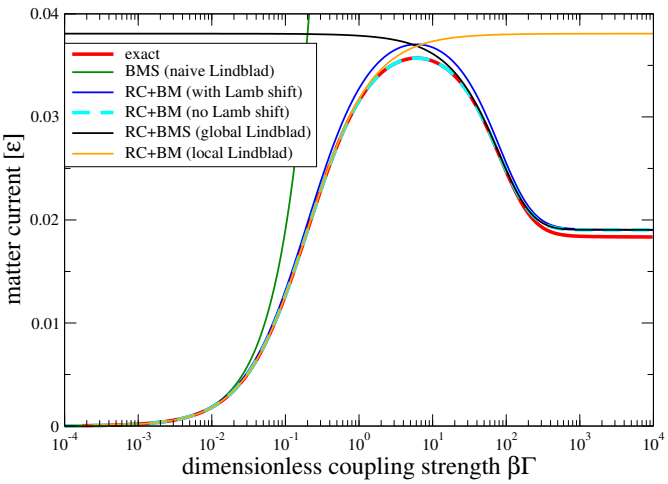

Figure 5.4: Plot of the matter current versus dimensionless coupling strength at a fixed non-equilibrium scenario. Lindblad approaches (green, black, orange) capture the exact solution (red) only in suitable regimes, whereas the Redfield master equation (light dashed blue and solid blue) recover the exact solution over various orders. In particular the naive SET Lindblad (green) captures only the weak-coupling regime. In contrast, the failure of the BMS for the TQD (black) fails at weak coupling since the secular approximation is not applicable. Parameters: $\Gamma_L = \Gamma_R = \Gamma$, $\beta_L\epsilon = \beta_R\epsilon = 1$, $\mu_L = +\epsilon$, $\mu_R = -\epsilon$, $\delta_L = \delta_R = 0.1\epsilon$, $\epsilon_L = \epsilon_R = \epsilon$.

Bibliography

[1] A. Nazir and G. Schaller. The reaction coordinate mapping in quantum thermodynamics. In F. Binder, L. A. Correa, C. Gogolin, J. Anders, and G. Adesso, editors, *Thermodynamics in the quantum regime – Recent progress and outlook*, Fundamental Theories of Physics, page 551. Springer, Cham, 2019.

[2] M. P. Woods, R. Groux, A. W. Chin, S. F. Huelga, and M. B. Plenio. Mappings of open quantum systems onto chain representations and Markovian embeddings. *Journal of Mathematical Physics*, 55:032101, 2014.

[3] Patrick P. Hofer, Martí Perarnau-Llobet, L. David, M. Miranda, Géraldine Haack, Ralph Silva, Jonatan Bohr Brask, and Nicolas Brunner. Markovian master equations for quantum thermal machines: local versus global approach. *New Journal of Physics*, 19:123037, 2017.