Open quantum systems – lecture 13

lecture
winter semester 2022/2023
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January 17, 2023

4.3 Quadratic models

We consider here time-independent (undriven) models, where the total Hamiltonian is a quadratic form of (bosonic or fermionic) system and bath annihilation and creation operators. Furthermore, we assume to start from a star-representation, where the reservoir modes do not couple to other reservoir modes, but only to system modes. In this case, the Heisenberg equations for the system operators read

$$\dot{\boldsymbol{d}}_i = \sum_k \alpha_{ij}\boldsymbol{d}_j + \sum_j \beta_{ij}\boldsymbol{d}_j^\dagger + \sum_k \gamma_{ik}\boldsymbol{c}_k + \sum_k \delta_{ik}\boldsymbol{c}_k^\dagger \,, \tag{4.1}$$

where the coefficients follow from the specifics of the model. When we compute the Heisenberg equations for the reservoir modes, we get

$$\dot{\boldsymbol{c}}_k = \sum_i \sigma_{ki}\boldsymbol{d}_i + \sum_i \kappa_{ki}\boldsymbol{d}_i^\dagger - \mathrm{i}\omega\boldsymbol{c}_k \,, \tag{4.2}$$

and analogous for the creation operators. We can now introduce Laplace-transformed operators

$$c_k(z) = \int_0^\infty \boldsymbol{c}_k e^{-zt}dt \,, \qquad \bar{c}_k(z) = \int_0^\infty \boldsymbol{c}_k^\dagger e^{-zt} \,, \tag{4.3}$$

and analogously for the system operators, which transforms the Heisenberg equations of motion into algebraic ones. In particular, due to the star-shaped structure we can solve the equations for the reservoir modes

$$zc_k(z) - c_k = \sum_i \sigma_{ki} d_i(z) + \sum_i \kappa_{ki}\bar{d}_i(z) - \mathrm{i}\omega c_k(z) \tag{4.4}$$

for $c_k(z)$ and insert the result into the other equations, thereby effectively eliminating all reservoir modes. Thereby, the problem is reduced to solving the equations for the system modes and then performing the inverse Laplace transform.

4.3.1 Bosonic model

We consider a harmonic oscillator coupled to multiple (later: infinitely many) bath oscillators

$$\begin{aligned} H &= \Omega a^\dagger a + \sum_k \omega_k \left[b_k^\dagger + \frac{h_k}{\omega_k}(a+a^\dagger)\right]\left[b_k + \frac{h_k^*}{\omega_k}(a+a^\dagger)\right] \\ &= \Omega a^\dagger a + \left(\sum_k \frac{\left|h_k\right|^2}{\omega_k}\right)(a+a^\dagger)^2 + (a+a^\dagger)\sum_k\left(h_k b_k + h_k^* b_k^\dagger\right) + \sum_k \omega_k b_k^\dagger b_k \,, \end{aligned} \tag{4.5}$$

where a and b_k are bosonic operators on the system and bath, respectively. In particular, we note that we have assumed a global Hamiltonian that maintains a lower spectral bound at all values of the coupling strength h_k, which upon expansion leads to a renormalization term for the system that is often neglected in the weak coupling limit. Without this term, the model should only be considered for weak couplings (cf. our derivation of the master equation).

We will now consider the Heisenberg equations of motion $\dot{\boldsymbol{O}} = \mathrm{i}[\boldsymbol{H}, \boldsymbol{O}]$ for operators O denoted by bold symbols in the Heisenberg picture. Since the total Hamiltonian is quadratic, these equations close with

$$
\begin{aligned}
\dot{\boldsymbol{a}} &= -\mathrm{i}\Omega\boldsymbol{a} - 2\mathrm{i}\left(\sum_k \frac{|h_k|^2}{\omega_k}\right)(\boldsymbol{a}+\boldsymbol{a}^\dagger) - \mathrm{i}\sum_k \left(h_k \boldsymbol{b_k} + h_k^* \boldsymbol{b_k^\dagger}\right) , \\
\dot{\boldsymbol{a}}^\dagger &= +\mathrm{i}\Omega\boldsymbol{a}^\dagger + 2\mathrm{i}\left(\sum_k \frac{|h_k|^2}{\omega_k}\right)(\boldsymbol{a}+\boldsymbol{a}^\dagger) + \mathrm{i}\sum_k \left(h_k \boldsymbol{b_k} + h_k^* \boldsymbol{b_k^\dagger}\right) , \\
\dot{\boldsymbol{b}}_{\boldsymbol{k}} &= -\mathrm{i}h_k^*(\boldsymbol{a}+\boldsymbol{a}^\dagger) - \mathrm{i}\omega_k \boldsymbol{b_k} , \\
\dot{\boldsymbol{b}}_{\boldsymbol{k}}^\dagger &= +\mathrm{i}h_k(\boldsymbol{a}+\boldsymbol{a}^\dagger) + \mathrm{i}\omega_k \boldsymbol{b_k^\dagger} .
\end{aligned}
\tag{4.6}
$$

In the decoupled limit $h_k \to 0$, this reproduces the expected simple isolated equations of motion. In the naive approach, we would have neglected the energy renormalization $\propto \left(\sum_k \frac{|h_k|^2}{\omega_k}\right)$. One could also obtain a formally exact solution then, but this may then lead (beyond a certain coupling strength) to a divergent position and momentum (not shown). Therefore, we proceed with the energy renormalization included. To rewrite the equations a bit, we use dimensionless position $\boldsymbol{x} = \boldsymbol{a}^\dagger + \boldsymbol{a}$ and momentum $\boldsymbol{p} = \mathrm{i}(\boldsymbol{a}^\dagger - \boldsymbol{a})$ operators, which leads to

$$
\begin{aligned}
\dot{\boldsymbol{x}} &= +\Omega\boldsymbol{p} , \\
\dot{\boldsymbol{p}} &= -\Omega\boldsymbol{x} - 4\left(\sum_k \frac{|h_k|^2}{\omega_k}\right)\boldsymbol{x} - 2\sum_k \left(h_k \boldsymbol{b_k} + h_k^* \boldsymbol{b_k^\dagger}\right) , \\
\dot{\boldsymbol{b}}_{\boldsymbol{k}} &= -\mathrm{i}h_k^*\boldsymbol{x} - \mathrm{i}\omega_k \boldsymbol{b_k} , \\
\dot{\boldsymbol{b}}_{\boldsymbol{k}}^\dagger &= +\mathrm{i}h_k\boldsymbol{x} + \mathrm{i}\omega_k \boldsymbol{b_k^\dagger} .
\end{aligned}
\tag{4.7}
$$

We can now introduce the Laplace-transformed operators

$$
\begin{aligned}
x(z) &= \int_0^\infty \boldsymbol{x} e^{-zt} dt , \qquad p(z) = \int_0^\infty \boldsymbol{p} e^{-zt} dt , \\
b_k(z) &= \int_0^\infty \boldsymbol{b_k} e^{-zt} dt , \qquad \bar{b}_k(z) = \int_0^\infty \boldsymbol{b_k^\dagger} e^{-zt} dt ,
\end{aligned}
\tag{4.8}
$$

which has the advantage of yielding an algebraic system

$$
\begin{aligned}
zx(z) - (a^\dagger + a) &= +\Omega p(z) , \\
zp(z) - \mathrm{i}(a^\dagger - a) &= -\Omega x(z) - 4\left(\sum_k \frac{|h_k|^2}{\omega_k}\right)x(z) - 2\sum_k \left(h_k b_k(z) + h_k^* \bar{b}_k(z)\right) , \\
zb_k(z) - b_k &= -\mathrm{i}h_k^* x(z) - \mathrm{i}\omega_k b_k(z) , \\
z\bar{b}_k(z) - b_k^\dagger &= +\mathrm{i}h_k x(z) + \mathrm{i}\omega_k \bar{b}_k(z) .
\end{aligned}
\tag{4.9}
$$

Thanks to the simple structure, we can express the reservoir operators and the position operator of the system in terms of the Laplace-transformed momentum operator and the initial operators

$$\begin{aligned}
x(z) &= \frac{a+a^\dagger}{z} + \frac{\Omega}{z} p(z)\,,\\
b_k(z) &= \frac{b_k}{z+\mathrm{i}\omega_k} - \frac{\mathrm{i}h_k^*}{z+\mathrm{i}\omega_k} x(z) = \frac{b_k}{z+\mathrm{i}\omega_k} - \frac{\mathrm{i}h_k^*}{z(z+\mathrm{i}\omega_k)}(a+a^\dagger) - \frac{\mathrm{i}h_k^*\Omega}{z(z+\mathrm{i}\omega_k)} p(z)\,,\\
\bar{b}_k(z) &= \frac{b_k^\dagger}{z-\mathrm{i}\omega_k} + \frac{\mathrm{i}h_k}{z-\mathrm{i}\omega_k} x(z) = \frac{b_k^\dagger}{z-\mathrm{i}\omega_k} + \frac{\mathrm{i}h_k}{z(z-\mathrm{i}\omega_k)}(a+a^\dagger) + \frac{\mathrm{i}h_k\Omega}{z(z-\mathrm{i}\omega_k)} p(z)\,,
\end{aligned} \tag{4.10}$$

such that we obtain a single equation for the momentum

$$\begin{aligned}
zp(z) = \mathrm{i}(a^\dagger - a) &+ \left[-\frac{\Omega}{z} - \frac{4}{z}\left(\sum_k \frac{|h_k|^2}{\omega_k}\right) + 2\mathrm{i}\sum_k \frac{|h_k|^2}{z(z+\mathrm{i}\omega_k)} - 2\mathrm{i}\sum_k \frac{|h_k|^2}{z(z-\mathrm{i}\omega_k)}\right](a+a^\dagger)\\
&- \sum_k \left[\frac{2h_k}{z+\mathrm{i}\omega_k}\right] b_k - \sum_k \left[\frac{2h_k^*}{z-\mathrm{i}\omega_k}\right] b_k^\dagger\\
&+ \left[-\frac{\Omega^2}{z} - \frac{4\Omega}{z}\left(\sum_k \frac{|h_k|^2}{\omega_k}\right) + 2\mathrm{i}\sum_k \frac{|h_k|^2\Omega}{z(z+\mathrm{i}\omega_k)} - 2\mathrm{i}\sum_k \frac{|h_k|^2\Omega}{z(z-\mathrm{i}\omega_k)}\right] p(z)\\
= \mathrm{i}(a^\dagger - a) &+ \left[-\frac{\Omega}{z} - \frac{4}{z}\left(\sum_k \frac{|h_k|^2}{\omega_k}\right) + 4\sum_k \frac{|h_k|^2\omega_k}{z(z^2+\omega_k^2)}\right](a+a^\dagger)\\
&- \sum_k \left[\frac{2h_k}{z+\mathrm{i}\omega_k}\right] b_k - \sum_k \left[\frac{2h_k^*}{z-\mathrm{i}\omega_k}\right] b_k^\dagger\\
&+ \left[-\frac{\Omega^2}{z} - \frac{4\Omega}{z}\left(\sum_k \frac{|h_k|^2}{\omega_k}\right) + 4\sum_k \frac{|h_k|^2\Omega\omega_k}{z(z^2+\omega_k^2)}\right] p(z)
\end{aligned} \tag{4.11}$$

We can already make some statements about the stationary limit of the above operators (or at least their period average) by considering the limits $\lim_{z\to 0} zp(z) = 0$, $\lim_{z\to 0} zx(z)$, $\lim_{z\to 0} zb_k(z) = 0$, and $\lim_{z\to 0} z\bar{b}_k(z) = 0$. To proceed further, it is necessary to specify a spectral function of the reservoir $\Gamma(\omega) = 2\pi\sum_k |h_k|^2\delta(\omega-\omega_k)$.

One option for such a spectral function (which leads to comparably simple results) is

$$\Gamma(\omega) = \Gamma\frac{\omega\delta^2}{\omega^2+\delta^2}\,, \tag{4.12}$$

where the dimensionless $\Gamma \geq 0$ quantifies the coupling strength and the spectral density becomes linear as $\delta \to \infty$. For this spectral density, we can perform all frequency integrals, yielding under the same initial conditions the equations

$$\begin{aligned}
z\left\langle p(z)\right\rangle &= p_0 + \frac{1}{z}\left[-\Omega - \Gamma\delta + \frac{\Gamma\delta^2}{z+\delta}\right] x_0 + \frac{\Omega}{z}\left[-\Omega - \Gamma\delta + \frac{\Gamma\delta^2}{z+\delta}\right]\left\langle p(z)\right\rangle\,,\\
\left\langle x(z)\right\rangle &= \frac{x_0}{z} + \frac{\Omega}{z}\left\langle p(z)\right\rangle\,,
\end{aligned} \tag{4.13}$$

which can be solved exactly for the momentum and position (yielding lengthy expressions through). In the weak-coupling and Markovian limit (small Γ and large δ), the master equation solution

$$\begin{aligned}
x(t) &= \exp\{-\Gamma(\Omega)t/2\}[\cos(\Omega t)x_0 + \sin(\Omega t)p_0]\,,\\
p(t) &= \exp\{-\Gamma(\Omega)t/2\}[\cos(\Omega t)p_0 - \sin(\Omega t)x_0]
\end{aligned} \tag{4.14}$$

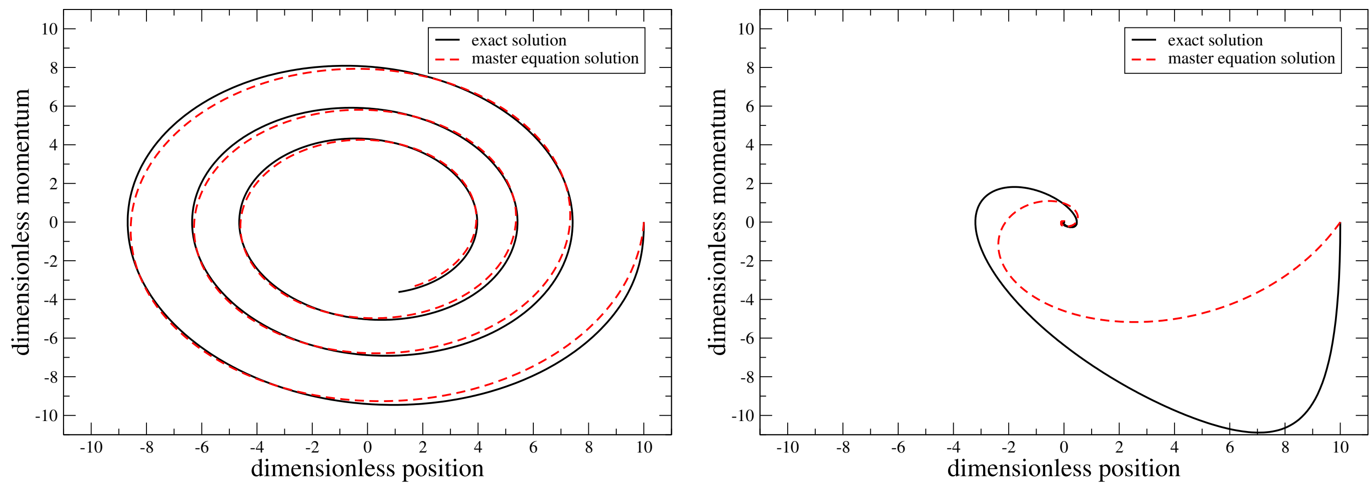

Figure 4.1: Parametric phase space plot of the exact solution (solid black) and the corresponding approximate master equation solution (dashed red). In the weak coupling limit (left, for $\Gamma = 0.1$), both agree well, although the pace is slightly different. In the strong coupling regime (right, for $\Gamma = 1.0$), significant differences appear. Other parameters: $\Omega t \in [0, 20]$, $x_0 = 10$, $p_0 = 0$, $\delta = 10\Omega$.

is reproduced, see Fig. 4.1. In the strong-coupling limit however, significant differences are visible. In particular, initially the distance between the steady state solution (origin) and the exact time-dependent solution even increases (non-Markovian signature).

We can also use this to compute other operators like e.g. $a^\dagger a = \frac{p^2+x^2}{4} - \frac{1}{2}$.

4.3.2 Fermionic transport: the SET

An important class for benchmarking perturbative approaches are exactly solvable models, where the total Hamiltonian is a quadratic form of bosonic or fermionic annihilation and creation operators. For example, the Fano Anderson model (SET) can be solved along a similar route as the SRL. The system, bath, and interaction Hamiltonians are given by

$$H_S = \epsilon d^\dagger d\,, \qquad H_B = \sum_k \epsilon_{kL} c_{kL}^\dagger c_{kL} + \sum_k \epsilon_{kR} c_{kR}^\dagger c_{kR}\,,$$
$$H_I = \sum_k \left(t_{kL} d c_{kL}^\dagger + t_{kL}^* c_{kL} d^\dagger \right) + \sum_k \left(t_{kR} d c_{kR}^\dagger + t_{kR}^* c_{kR} d^\dagger \right)\,, \tag{4.15}$$

where d is a fermionic annihilation operator on the dot and $c_{k\nu}$ are fermionic annihilation operators of an electron in the k-th mode of lead ν. Obviously, this corresponds to a quadratic fermionic Hamiltonian, which can in principle be solved exactly by various methods such as e.g. non-equilibrium Greens functions [1] or even the equation-of-motion approach [2]. Such quadratic models are useful to study exact transport properties [3] or exact master equations [4].

Heisenberg Picture Dynamics

To be as self-contained as possible, we here simply compute the Heisenberg equations of motion for the system and bath annihilation operators (we denote operators in the Heisenberg picture by boldface symbols)

$$\begin{aligned}
\dot{\boldsymbol{d}} &= -\mathrm{i}\epsilon\boldsymbol{d} + \mathrm{i}\sum_k \left[t_{kL}^* \boldsymbol{c_{kL}} + t_{kR}^* \boldsymbol{c_{kR}}\right] ,\\
\dot{\boldsymbol{c}}_{kL} &= -\mathrm{i}\epsilon_{kL}\boldsymbol{c_{kL}} + \mathrm{i}t_{kL}\boldsymbol{d}\,, \qquad \dot{\boldsymbol{c}}_{kR} = -\mathrm{i}\epsilon_{kR}\boldsymbol{c_{kR}} + \mathrm{i}t_{kR}\boldsymbol{d}\,.
\end{aligned} \tag{4.16}$$

Surprisingly, this system is already closed and we obtain its solution by performing a Laplace transform [5]

$$\begin{aligned}
zd(z) - d &= -\mathrm{i}\epsilon d(z) + \mathrm{i}\sum_k \left[t_{kL}^* c_{kL}(z) + t_{kR}^* c_{kR}(z)\right] ,\\
zc_{kL}(z) - c_{kL} &= -\mathrm{i}\epsilon_{kL}c_{kL}(z) + \mathrm{i}t_{kL}d(z)\,, \qquad zc_{kR}(z) - c_{kR} = -\mathrm{i}\epsilon_{kR}c_{kR}(z) + \mathrm{i}t_{kR}d(z)\,.
\end{aligned} \tag{4.17}$$

In the above equations, we can eliminate the operators $c_{kL}(z)$ and $c_{kR}(z)$ as before. This yields for the dot annihilation operator

$$d(z) = \frac{d + \mathrm{i}\sum_k \left(\frac{t_{kL}^* c_{kL}}{z+\mathrm{i}\epsilon_{kL}} + \frac{t_{kR}^* c_{kR}}{z+\mathrm{i}\epsilon_{kR}}\right)}{z + \mathrm{i}\epsilon + \sum_k \left(\frac{|t_{kL}|^2}{z+\mathrm{i}\epsilon_{kL}} + \frac{|t_{kR}|^2}{z+\mathrm{i}\epsilon_{kR}}\right)} \equiv f(z)d + \sum_k \left(g_{kL}(z)c_{kL} + g_{kR}(z)c_{kR}\right) , \tag{4.18}$$

where we have introduced the functions $g_{k\nu}(z)$ and $f(z)$. This expression also yields the solution for the operators of the right lead modes

$$c_{k\nu}(z) = \frac{1}{z + \mathrm{i}\epsilon_{k\nu}} c_{k\nu} + \frac{\mathrm{i}t_{k\nu}}{z + \mathrm{i}\epsilon_{k\nu}} d(z)\,. \tag{4.19}$$

Inverting the Laplace transform may now be achieved by identifying the poles and applying the residue theorem. In the wide-band limit discussed below, this becomes particularly simple.

Asymptotic evolution

To find the full time evolution of the operators in the Heisenberg picture, we have to compute the inverse Laplace transform of

$$\begin{aligned}
f(z) &= \frac{1}{z + \mathrm{i}\epsilon + \sum_k \left(\frac{|t_{kL}|^2}{z+\mathrm{i}\epsilon_{kL}} + \frac{|t_{kR}|^2}{z+\mathrm{i}\epsilon_{kR}}\right)} ,\\
g_{k\nu}(z) &= \frac{\mathrm{i}t_{k\nu}^*}{\left[z + \mathrm{i}\epsilon_{k\nu}\right]\left[z + \mathrm{i}\epsilon + \sum_k \left(\frac{|t_{kL}|^2}{z+\mathrm{i}\epsilon_{kL}} + \frac{|t_{kR}|^2}{z+\mathrm{i}\epsilon_{kR}}\right)\right]} ,
\end{aligned} \tag{4.20}$$

which heavily depends on the number of modes and their distribution in the reservoir. Any system with a finite number of reservoir modes, for example, will exhibit recurrences to the initial state.

Only systems with a continuous spectrum of reservoir modes can be expected to yield a stationary system state. To obtain that limit, we approximate the summation over discrete modes by an integral formally by introducing the energy-dependent **tunnel rate** or **spectral density**

$$\Gamma_\nu(\omega) = 2\pi \sum_k |t_{k\nu}|^2 \delta(\omega - \epsilon_{k\nu})\,. \tag{4.21}$$

To obtain simple results, we will specifically assume a Lorentzian-shaped tunneling rate [6]

$$\Gamma_\nu(\omega) = \frac{\Gamma_\nu \delta_\nu^2}{\omega^2 + \delta_\nu^2}\,. \tag{4.22}$$

The simple pole structure of such tunneling rates renders analytic calculations simple. Superpositions of many Lorentzian shapes with shifted centers may approximate quite general tunneling rates [7]. With this, we get

$$\begin{aligned}
f(z) &\approx \frac{1}{z + \mathrm{i}\epsilon + \int \frac{1}{2\pi}\left(\frac{\Gamma_L \delta_L^2}{\omega^2+\delta_L^2} + \frac{\Gamma_R \delta_R^2}{\omega^2+\delta_R^2}\right)\frac{1}{z+\mathrm{i}\omega} d\omega} = \frac{1}{z + \mathrm{i}\epsilon + \frac{1}{2}\left(\frac{\Gamma_L\delta_L}{z+\delta_L} + \frac{\Gamma_R\delta_R}{z+\delta_R}\right)}\,,\\
g_{k\nu}(z) &\approx \frac{\mathrm{i}t_{k\nu}^*}{(z+\mathrm{i}\epsilon_{k\nu})\left[z + \mathrm{i}\epsilon + \int \frac{1}{2\pi}\left(\frac{\Gamma_L \delta_L^2}{\omega^2+\delta_L^2} + \frac{\Gamma_R \delta_R^2}{\omega^2+\delta_R^2}\right)\frac{1}{z+\mathrm{i}\omega} d\omega\right]}\\
&= \frac{1}{[z+\mathrm{i}\epsilon_{k\nu}]\left[z + \mathrm{i}\epsilon + \frac{1}{2}\left(\frac{\Gamma_L\delta_L}{z+\delta_L} + \frac{\Gamma_R\delta_R}{z+\delta_R}\right)\right]}\,.
\end{aligned} \tag{4.23}$$

To obtain sufficiently simple results, we assume the **wide-band limit** $\delta_\nu \to \infty$ (within which the tunneling rates are flat), where one obtains the simple expression

$$\begin{aligned}
f(z) &\to \frac{1}{z + \mathrm{i}\epsilon + (\Gamma_L + \Gamma_R)/2}\,,\\
g_{k\nu}(z) &\to \frac{\mathrm{i}t_{k\nu}^*}{(z+\mathrm{i}\epsilon_{k\nu})\left[z + \mathrm{i}\epsilon + (\Gamma_L+\Gamma_R)/2\right]}\,.
\end{aligned} \tag{4.24}$$

Inserting the inverse Laplace transforms of these expressions

$$\begin{aligned}
f(t) &\to e^{-\mathrm{i}\epsilon t} e^{-\Gamma t/2}\,,\\
g_{k\nu}(t) &\to \frac{t_{k\nu}^*\left(e^{-\mathrm{i}\epsilon t}e^{-\Gamma t/2} - e^{-\mathrm{i}\epsilon_{k\nu} t}\right)}{\epsilon_{k\nu} - \epsilon + \mathrm{i}\Gamma/2}
\end{aligned} \tag{4.25}$$

(with $\Gamma \equiv \Gamma_L + \Gamma_R$) into the equations for the dot then yields in the long-term limit

$$\boldsymbol{d(t)} = \sum_k g_{kL}(t) c_{kL} + \sum_k g_{kR}(t) c_{kR} \tag{4.26}$$

allows to express the dot Heisenberg operator in terms of the initial or Schrödinger picture operators.

Specifically, we get in the long-term limit

$$\boldsymbol{d(t)} \to -\sum_k \frac{t_{kL}^* e^{-\mathrm{i}\epsilon_{kL} t}}{\epsilon_{kL} - \epsilon + \mathrm{i}\Gamma/2} c_{kL} - \sum_k \frac{t_{kR}^* e^{-\mathrm{i}\epsilon_{kR} t}}{\epsilon_{kR} - \epsilon + \mathrm{i}\Gamma/2} c_{kR}\,, \tag{4.27}$$

where we see that asymptotically, the initial occupation of the dot is not relevant.

Using Eq. (4.19), also the right lead modes can be expressed in terms of the Schrödinger picture operators

$$\begin{aligned}
c_{kR}(z) = &\frac{\mathrm{i}t_{kR}}{(z+\mathrm{i}\epsilon_{kR})(z+\mathrm{i}\epsilon+\Gamma/2)} d + \frac{1}{z+\mathrm{i}\epsilon_{kR}} c_{kR}\\
&- \sum_q \frac{t_{kR}t_{qL}^*}{(z+\mathrm{i}\epsilon_{kR})(z+\mathrm{i}\epsilon_{qL})(z+\mathrm{i}\epsilon+\Gamma/2)} c_{qL}\\
&- \sum_q \frac{t_{kR}t_{qR}^*}{(z+\mathrm{i}\epsilon_{kR})(z+\mathrm{i}\epsilon_{qR})(z+\mathrm{i}\epsilon+\Gamma/2)} c_{qR}\,.
\end{aligned} \tag{4.28}$$

Now, performing the inverse Laplace transform and neglecting all transient dynamics, we obtain the asymptotic evolution of the annihilation operators in the Heisenberg picture

$$\begin{aligned}\boldsymbol{c}_{kR}(t) \to & \left(-\frac{t_{kR}e^{-\mathrm{i}\epsilon_{kR}t}}{\epsilon_{kR}-\epsilon+\mathrm{i}\Gamma/2}\right)d + e^{-\mathrm{i}\epsilon_{kR}t}c_{kR} \\ & + \sum_q \frac{t_{kR}t_{qL}^*}{\epsilon_{kR}-\epsilon_{qL}}\left(\frac{e^{-\mathrm{i}\epsilon_{qL}t}}{\epsilon_{qL}-\epsilon+\mathrm{i}\Gamma/2} - \frac{e^{-\mathrm{i}\epsilon_{kR}t}}{\epsilon_{kR}-\epsilon+\mathrm{i}\Gamma/2}\right)c_{qL} \\ & + \sum_q \frac{t_{kR}t_{qR}^*}{\epsilon_{kR}-\epsilon_{qR}}\left(\frac{e^{-\mathrm{i}\epsilon_{qR}t}}{\epsilon_{qR}-\epsilon+\mathrm{i}\Gamma/2} - \frac{e^{-\mathrm{i}\epsilon_{kR}t}}{\epsilon_{kR}-\epsilon+\mathrm{i}\Gamma/2}\right)c_{qR}\,. \end{aligned} \tag{4.29}$$

Time-dependent and stationary occupation

The full time-dependent occupation $n(t) = \left\langle d^\dagger(t)d(t)\right\rangle$ is found by inverting the Laplace transform. For the moment we do it formally and already perform the expectation value

$$\begin{aligned} n(t) &= \left\langle \left[f^*(t)d^\dagger + \sum_k \left(g_{kL}^*(t)c_{kL}^\dagger + g_{kR}^*(t)c_{kR}^\dagger\right)\right]\left[f(t)d + \sum_k \left(g_{kL}(t)c_{kL} + g_{kR}(t)c_{kR}\right)\right]\right\rangle \\ &= |f(t)|^2 n_0 + \sum_k \left(|g_{kL}(t)|^2 f_L(\epsilon_{kL}) + |g_{kR}(t)|^2 f_R(\epsilon_{kR})\right)\,, \end{aligned} \tag{4.30}$$

where we have used a product state as an initial one

$$\rho_0 = \rho_S^0 \frac{e^{-\beta_L(H_L-\mu_L N_L)}}{Z_L}\frac{e^{-\beta_R(H_R-\mu_R N_R)}}{Z_R} \tag{4.31}$$

with the lead Hamiltonians $H_\nu = \sum_k \epsilon_{k\nu}c_{k\nu}^\dagger c_{k\nu}$ and the lead particle numbers $N_\nu = \sum_k c_{k\nu}^\dagger c_{k\nu}$. These eventually yield the only non-vanishing expectation values $n_0 = \left\langle d^\dagger d\right\rangle$ and $f_\nu(\epsilon_{k\nu}) = \left\langle c_{k\nu}^\dagger c_{k\nu}\right\rangle$. Inverse lead temperatures β_ν and chemical potentials μ_ν thereby only enter implicitly in the Fermi functions.

we obtain by switching to a continuum representation

$$\begin{aligned} n(t) &= e^{-\Gamma t}n_0 + \sum_k\sum_\nu |t_{k\nu}|^2 f_\nu(\epsilon_{k\nu}) 4\frac{1-2e^{-\Gamma t/2}\cos[(\epsilon_{k\nu}-\epsilon)t]+e^{-\Gamma t}}{\Gamma^2+4(\epsilon_{k\nu}-\epsilon)^2} \\ &= e^{-\Gamma t}n_0 + \sum_\nu \int d\omega \Gamma_\nu f_\nu(\omega)\frac{4}{2\pi}\frac{1-2e^{-\Gamma t/2}\cos[(\omega-\epsilon)t]+e^{-\Gamma t}}{\Gamma^2+4(\omega-\epsilon)^2}\,. \end{aligned} \tag{4.32}$$

The long-term limit can – due to $\Gamma > 0$ – be determined easily, and the stationary occupation becomes

$$\bar{n} = \sum_\nu \int d\omega \Gamma_\nu f_\nu(\omega)\frac{2}{\pi}\frac{1}{\Gamma^2+4(\omega-\epsilon)^2}\,. \tag{4.33}$$

With the above formula for the stationary occupation valid for the wide-band limit, one can easily demonstrate the following:

- At infinite bias $f_L(\omega) = 1$ and $f_R(\omega) = 0$, the stationary occupation approaches $\bar{n} \to \Gamma_L/(\Gamma_L+\Gamma_R)$, regardless of the coupling strength. A similar result is of course obtained for reverse infinite bias where $\bar{n} \to \Gamma_R/(\Gamma_L+\Gamma_R)$.

- When the quantum dot is coupled weakly to a single bath only (e.g. $\Gamma_R(\omega) = 0$), the stationary occupation approaches the Fermi distribution of the coupled lead, evaluated at the dot energy (e.g. $\bar{n} = f_L(\epsilon) + \mathcal{O}\{\Gamma_L\}$). This implies that for weak coupling to an equilibrium reservoir, the system will equilibrate with the temperature and chemical potential of the reservoir, consistent with what one expects from a master equation approach.

- When the dot is coupled weakly to both reservoirs, the stationary state approaches

$$\bar{n} \to \frac{\Gamma_L f_L(\epsilon) + \Gamma_R f_R(\epsilon)}{\Gamma_L + \Gamma_R}\,, \tag{4.34}$$

  which is also obtained within a master equation approach. By using that $\delta(x) = \lim_{\epsilon\to 0} \frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2}$, one can show that also formally.

- In contrast, for the strong-coupling limit, the stationary occupation will be suppressed $\bar{n} \to 0$, as the exact solution for the stationary state is no longer localized on the dot.

Stationary Current

For simplicity, we will only consider the stationary current from left to right here. It can be defined as the long-term limit of the change of particle numbers at the right lead

$$I_M = \lim_{t\to\infty} \frac{d}{dt}\left\langle \sum_k c_{kR}^\dagger c_{kR}\right\rangle = -\lim_{t\to\infty}\frac{d}{dt}\left\langle \sum_k c_{kL}^\dagger c_{kL}\right\rangle\,, \tag{4.35}$$

which we can evaluate in the Heisenberg picture as we did for the stationary occupation

$$I = \mathrm{i}\sum_k t_{kR}\left\langle \boldsymbol{c}_{\boldsymbol{kR}}^\dagger(t)\boldsymbol{d}(t)\right\rangle + \text{h.c.}\,. \tag{4.36}$$

The r.h.s. of the above equation is also known as **current operator**.

From Eq. (4.29) we can obtain the long-term asymptotic evolution of the right lead occupation

$$\begin{aligned}
N_R \to & \sum_k \frac{|t_{kR}|^2}{(\epsilon_{kR}-\epsilon)^2+\Gamma^2/4} n_0 + N_R^0 \\
& - \sum_{kq}\left[\frac{t_{kR}t_{qR}^*}{\epsilon_{kR}-\epsilon_{qR}} e^{+\mathrm{i}\epsilon_{kR}t}\left(\frac{e^{-\mathrm{i}\epsilon_{qR}t}}{\epsilon_{qR}-\epsilon+\mathrm{i}\Gamma/2} - \frac{e^{-\mathrm{i}\epsilon_{kR}t}}{\epsilon_{kR}-\epsilon+\mathrm{i}\Gamma/2}\right)\delta_{kq} f_R(\epsilon_{kR}) + \text{h.c.}\right] \\
& + \sum_{kq}\frac{|t_{kR}|^2|t_{qL}|^2}{(\epsilon_{kR}-\epsilon_{qL})^2}\left(\frac{e^{+\mathrm{i}\epsilon_{qL}t}}{\epsilon_{qL}-\epsilon-\mathrm{i}\Gamma/2} - \frac{e^{+\mathrm{i}\epsilon_{kR}t}}{\epsilon_{kR}-\epsilon-\mathrm{i}\Gamma/2}\right) \\
& \quad\times\left(\frac{e^{-\mathrm{i}\epsilon_{qL}t}}{\epsilon_{qL}-\epsilon+\mathrm{i}\Gamma/2} - \frac{e^{-\mathrm{i}\epsilon_{kR}t}}{\epsilon_{kR}-\epsilon+\mathrm{i}\Gamma/2}\right) f_L(\epsilon_{qL}) \\
& + \sum_{kq}\frac{|t_{kR}|^2|t_{qR}|^2}{(\epsilon_{kR}-\epsilon_{qR})^2}\left(\frac{e^{+\mathrm{i}\epsilon_{qR}t}}{\epsilon_{qR}-\epsilon-\mathrm{i}\Gamma/2} - \frac{e^{+\mathrm{i}\epsilon_{kR}t}}{\epsilon_{kR}-\epsilon-\mathrm{i}\Gamma/2}\right) \\
& \quad\times\left(\frac{e^{-\mathrm{i}\epsilon_{qR}t}}{\epsilon_{qR}-\epsilon+\mathrm{i}\Gamma/2} - \frac{e^{-\mathrm{i}\epsilon_{kR}t}}{\epsilon_{kR}-\epsilon+\mathrm{i}\Gamma/2}\right) f_R(\epsilon_{qR})\,.
\end{aligned} \tag{4.37}$$

Introducing the tunneling rates in the wide-band limit $\Gamma_\nu \approx \Gamma_\nu(\omega) = 2\pi \sum_k |t_{k\nu}|^2 \delta(\omega - \epsilon_{k\nu})$, we can represent the right lead occupation by integrals

$$N_R \to \frac{1}{2\pi}\int d\omega \frac{\Gamma_R}{(\omega-\epsilon)^2+\Gamma^2/4} n_0 + N_R^0 - \frac{1}{2\pi}\int d\omega \Gamma_R f_R(\omega)\left[\frac{4+4\mathrm{i}\omega t - 2t(\Gamma+2\mathrm{i}\epsilon)}{(2\omega+\mathrm{i}\Gamma-2\epsilon)^2} + \text{h.c.}\right]$$
$$+ \frac{1}{4\pi^2}\int d\omega d\omega' \left(\Gamma_L\Gamma_R f_L(\omega') + \Gamma_R^2 f_R(\omega')\right)\frac{1}{(\omega-\omega')^2}\left|\frac{e^{-\mathrm{i}\omega' t}}{\omega'-\epsilon+\mathrm{i}\Gamma/2} - \frac{e^{-\mathrm{i}\omega t}}{\omega-\epsilon+\mathrm{i}\Gamma/2}\right|^2 . \quad (4.38)$$

Whereas the first two terms are constant and do not contribute to the current, all other terms yield a non-vanishing contribution. The long-term limit of the time-derivative of the very last term is a bit involved to determine. It can be found, for example, by using properties of the Laplace transform. To evaluate the current, we therefore consider the limit

$$\begin{aligned}
F(\omega') &\equiv \lim_{t\to\infty}\frac{d}{dt}\int d\omega \frac{1}{(\omega-\omega')^2}\left|\frac{e^{-\mathrm{i}\omega' t}}{\omega'-\epsilon+\mathrm{i}\Gamma/2} - \frac{e^{-\mathrm{i}\omega t}}{\omega-\epsilon+\mathrm{i}\Gamma/2}\right|^2 \\
&= \lim_{z\to 0} z\int_0^\infty dt e^{-zt}\frac{d}{dt}\int d\omega \frac{1}{(\omega-\omega')^2}\left|\frac{e^{-\mathrm{i}\omega' t}}{\omega'-\epsilon+\mathrm{i}\Gamma/2} - \frac{e^{-\mathrm{i}\omega t}}{\omega-\epsilon+\mathrm{i}\Gamma/2}\right|^2 \\
&= \frac{8\pi}{\Gamma^2+4(\omega'-\epsilon)^2} , \qquad (4.39)
\end{aligned}$$

which with its Lorentzian shape converges for small Γ towards a Dirac-Delta distribution. Eventually, the current becomes

$$\begin{aligned}
I_M &= -\frac{1}{\pi}\int d\omega \Gamma_R f_R(\omega)\frac{\Gamma/2}{(\omega-\epsilon)^2+(\Gamma/2)^2} + \frac{1}{\pi\Gamma}\int d\omega \left(\Gamma_L\Gamma_R f_L(\omega) + \Gamma_R^2 f_R(\omega)\right)\frac{\Gamma/2}{(\omega-\epsilon)^2+(\Gamma/2)^2} \\
&= \frac{\Gamma_L\Gamma_R}{\Gamma_L+\Gamma_R}\int d\omega \left[f_L(\omega)-f_R(\omega)\right]\frac{1}{\pi}\frac{\Gamma/2}{(\omega-\epsilon)^2+(\Gamma/2)^2} . \qquad (4.40)
\end{aligned}$$

Comparing this with the **Landauer formula**, according to which the current can be expressed as $I_M = \frac{1}{2\pi}\int d\omega T(\omega)[f_L(\omega)-f_R(\omega)]$, we can read off the **transmission** of the SET in the wideband limit

$$T_{\rm SET}(\omega) = \frac{\Gamma_L\Gamma_R}{(\omega-\epsilon)^2+(\Gamma_L+\Gamma_R)^2/4} . \qquad (4.41)$$

The integrals in the above expression can be solved analytically by analysis in the complex plane, but here we will be content with the above integral representation, which can also be found using non-equilibrium Greens functions [1]. For consistency, we note that the current is antisymmetric under exchange of left and right leads as expected.

In the weak-coupling limit $\Gamma \to 0$, the current reduces to the known result

$$I_M = \frac{\Gamma_L\Gamma_R}{\Gamma_L+\Gamma_R}\left[f_L(\epsilon)-f_R(\epsilon)\right] , \qquad (4.42)$$

which at equal temperatures left and right implies that the current always flows from the lead with larger chemical potential to the one with lower chemical potential. This can be seen by using the representation of the Dirac-δ function as before.

Finally, we note further that, in the infinite bias limit ($f_L(\omega)\to 1$ and $f_R(\omega)\to 0$), the current becomes $I = \Gamma_L\Gamma_R/(\Gamma_L+\Gamma_R)$, which is independent of the coupling strength and also consistent

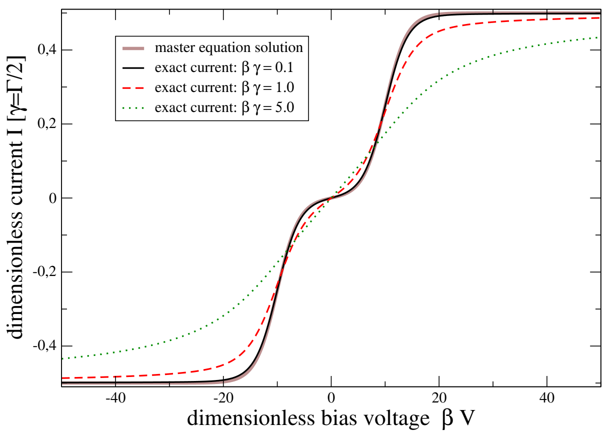

Figure 4.2: Plot of the electronic matter current (in units of $\gamma = \Gamma_L = \Gamma_R = \Gamma/2$) versus the bias voltage for symmetric tunneling rates and equal electronic temperatures $\beta_L = \beta_R = \beta$ and dot level $\beta\epsilon = 5$. For small coupling strength, exact (black solid) and master equation solution (brown bold) coincide for all bias voltages. For stronger couplings (red dashed and green dotted, respectively), the determination of the dot level ϵ from the current is no longer possible.

with Eq. (4.42). We have already seen that the master equation approach applied to the same problem reproduces Eq. (4.42) and therefore coincides with the exact result in the infinite bias limit.

Fig. 4.2 demonstrates the effect of increasing but symmetric coupling strengths $\Gamma_L = \Gamma_R = \gamma$ on the current. Whereas the weak-coupling result is well approximated when $\beta\gamma \ll 1$, one may observe significant deviations for strong couplings. In the shown example, spectroscopy of the dot level ϵ via detecting steps in the $I - V$ characteristics is therefore only possible in the weak-coupling limit.

An analogous result can be obtained for the stationary energy current $I_E = \frac{1}{2\pi}\int \omega T(\omega)[f_L(\omega) - f_R(\omega)]d\omega$, and one can show that for such Landauer-type transport, the second law is obeyed $(\beta_R - \beta_L)I_E + (\beta_L\mu_L - \beta_R\mu_R)I_M \geq 0$ [8].

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