Chapter 3
Exactly Solvable Models

Abstract To understand the limit within which master equations are valid, it is quite instructive to compare the master equation results against exactly solvable models. Unfortunately, these models are quite rare. In this chapter, we will discuss two popular representatives of exactly solvable models: first, we investigate a pure dephasing spin-boson model, where the interaction Hamiltonian commutes with the system Hamiltonian. Such models obviously leave the system energy invariant but nevertheless may be used to investigate interesting features such as decoherence. Second, we consider a noninteracting model, where the Hamiltonian can be written as a quadratic form of fermionic annihilation and creation operators. Such models generally admit—at least formally—an exact solution, and can thus be used to study non-equilibrium setups and transport in a regime where the coupling between system and reservoir becomes strong. Furthermore, we note that the non-equilibrium stationary solution of these models may also define a non-equilibrium reservoir.

3.1 Pure Dephasing Spin-Boson Model

The pure dephasing spin-boson model describes the interaction of a two-level system with a bosonic bath:

$$\begin{aligned} H_{\mathrm{S}} &= \omega\sigma^z, \\ H_{\mathrm{B}} &= \sum_k \omega_k \big(b_k^\dagger b_k + 1/2\big), \\ H_{\mathrm{I}} &= \sigma^z \otimes \sum_k \big(h_k b_k + h_k^* b_k^\dagger\big), \end{aligned} \tag{3.1}$$

where σ^z is a Pauli matrix and b_k a bosonic annihilation operator in the bath. One immediately observes that the model conserves the system energy—since $[H_{\mathrm{S}}, H_{\mathrm{I}}] = 0$—and will thus only modify the evolution of coherences in the system energy eigenbasis (hence the name purely dephasing). Similar models have been used to illustrate decoherence in quantum computers [1, 2] or to test the validity of Markovian master equations [3].

G. Schaller, *Open Quantum Systems Far from Equilibrium*, Lecture Notes in Physics 881,
DOI 10.1007/978-3-319-03877-3_3,

3.1.1 Time Evolution Operator

The calculation of the exact solution makes use of the fact that in the interaction picture, the time evolution operator can be exactly determined. In the interaction picture, the full density matrix follows the von Neumann equation

$$\dot{\boldsymbol{\rho}} = -\mathrm{i}\left[\boldsymbol{H}_{\mathrm{I}}(t), \boldsymbol{\rho}(t)\right] \tag{3.2}$$

with the interaction Hamiltonian in the interaction picture

$$\boldsymbol{H}_{\mathrm{I}}(t) = \sigma^z \otimes \sum_k \left(h_k b_k e^{-\mathrm{i}\omega_k \tau} + h_k^* b_k^\dagger e^{+\mathrm{i}\omega_k \tau}\right). \tag{3.3}$$

Exercise 3.1 (Interaction picture) Show that Eq. (3.3) arises in the interaction picture.

We note that the commutator of the interaction Hamiltonian with itself at different times is just a number,

$$\left[\boldsymbol{H}_{\mathrm{I}}(t_1), \boldsymbol{H}_{\mathrm{I}}(t_2)\right] = \sum_k |h_k|^2 2\mathrm{i} \sin\left[\omega_k(t_2 - t_1)\right], \tag{3.4}$$

such that the Baker–Campbell–Hausdorff (BCH) formula may be employed to calculate the exponential. For two operators A and B with the commutator obeying $[[A, B], A] = \mathbf{0} = [[A, B], B]$, one can express the exponential of the sum by a product of exponentials

$$e^{A+B} = e^A e^B e^{-[A,B]/2}. \tag{3.5}$$

If one now has many of these operators in the exponent $A_1, \ldots, A_n$ obeying $[A_i, A_j] = \alpha_{ij}\mathbf{1}$ such that $[[A_i, A_j], A_k] = \mathbf{0}$, one can generalize the above equation to

$$e^{\sum_{i=1}^n A_i} = e^{A_1} e^{A_2} \cdots e^{A_{n-1}} e^{A_n} e^{-\sum_{i<j}[A_i, A_j]/2}. \tag{3.6}$$

Exercise 3.2 (BCH formula) Show the generalization from Eq. (3.5) to Eq. (3.6).

Following the ideas in Ref. [3], we discretize the integral in the exponent of the time evolution operator:

$$\boldsymbol{U}(t) = \tau e^{-\mathrm{i}\int_0^t \boldsymbol{H}_{\mathrm{I}}(t')\,dt'} = \tau \lim_{\Delta t \to 0, N \to \infty} e^{\sum_{n=1}^N H_n \Delta t}, \tag{3.7}$$

where $H_n = -\mathrm{i}\boldsymbol{H}_{\mathrm{I}}(n\Delta t)$ with the constraint $N\Delta t = t$ remaining finite. Applying the generalized BCH formula (3.6), we obtain

$$\boldsymbol{U}(t) = \tau \prod_{n=1}^N e^{H_n \Delta t} e^{-\sum_{i<j}[H_i, H_j]/2} = \prod_{n=1}^N e^{H_n \Delta t} e^{-\sum_{i<j}[H_i, H_j]/2}, \tag{3.8}$$

where we note that the last exponential is just a number and that the operators are already time-ordered, such that the time ordering may simply be omitted. Recombining the exponentials of the operators, we see that the time ordering has no effect in this particular case:

$$\boldsymbol{U}(t) = e^{-\mathrm{i}\int_0^t \boldsymbol{H}_\mathrm{I}(t')\,dt'} = e^{\sigma^z \otimes \sum_k (\alpha_k(t) b_k - \alpha_k^*(t) b_k^\dagger)} \equiv e^{\sigma^z \otimes A(t)} \tag{3.9}$$

with $\alpha_k(t) = (e^{-\mathrm{i}\omega_k t} - 1)h_k/\omega_k$ and $A(t) = -A^\dagger(t)$.

Exercise 3.3 (Matrix exponentials) Show that for a unit vector $|\boldsymbol{n}| = 1$ and a vector of Pauli matrices $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ one has

$$e^{(\boldsymbol{n}\cdot\boldsymbol{\sigma})\otimes A} = \mathbf{1} \otimes \cosh(A) + (\boldsymbol{n} \cdot \boldsymbol{\sigma}) \otimes \sinh(A).$$

We can also write the unitary transformation as

$$\begin{aligned} \boldsymbol{U}(t) &= \mathbf{1} \otimes \frac{1}{2}\left(e^{+A(t)} + e^{-A(t)}\right) + \sigma^z \otimes \frac{1}{2}\left(e^{+A(t)} - e^{-A(t)}\right), \\ \boldsymbol{U}^\dagger(t) &= \mathbf{1} \otimes \frac{1}{2}\left(e^{+A(t)} + e^{-A(t)}\right) - \sigma^z \otimes \frac{1}{2}\left(e^{+A(t)} - e^{-A(t)}\right). \end{aligned} \tag{3.10}$$

When assuming an initial product state, the full density matrix is given by $\boldsymbol{\rho}(t) = \boldsymbol{U}(t)\rho_\mathrm{S}^0 \otimes \bar{\rho}_\mathrm{B}\boldsymbol{U}^\dagger(t)$, which can be used to calculate any expectation value.

3.1.2 Reduced Dynamics

By performing the partial trace over the reservoir, we obtain the exact solution in the interaction picture:

$$\begin{aligned} \boldsymbol{\rho}_\mathrm{S}(t) &= \mathrm{Tr}_\mathrm{B}\left\{\boldsymbol{U}(t)\rho_\mathrm{S}^0 \otimes \bar{\rho}_\mathrm{B}\boldsymbol{U}^\dagger(t)\right\} \\ &= \rho_\mathrm{S}^0 \frac{1}{4}\,\mathrm{Tr}_\mathrm{B}\left\{\left(e^{+2A(t)} + e^{-2A(t)} + 2\right)\bar{\rho}_\mathrm{B}\right\} \\ &\quad - \rho_\mathrm{S}^0\sigma^z \frac{1}{4}\,\mathrm{Tr}_\mathrm{B}\left\{\left(e^{+2A(t)} - e^{-2A(t)}\right)\bar{\rho}_\mathrm{B}\right\} \\ &\quad + \sigma^z\rho_\mathrm{S}^0 \frac{1}{4}\,\mathrm{Tr}_\mathrm{B}\left\{\left(e^{+2A(t)} - e^{-2A(t)}\right)\bar{\rho}_\mathrm{B}\right\} \\ &\quad - \sigma^z\rho_\mathrm{S}^0\sigma^z \frac{1}{4}\,\mathrm{Tr}_\mathrm{B}\left\{\left(e^{+2A(t)} + e^{-2A(t)} - 2\right)\bar{\rho}_\mathrm{B}\right\}, \end{aligned} \tag{3.11}$$

which can therefore be related to the expectation values $\langle e^{\pm 2A(t)}\rangle$ with respect to a thermal state. Since the bosonic annihilation and creation operators commute for different modes, we can separate the modes in the exponentials and write $\mathrm{Tr}_{\mathrm{B}}\{e^{2A(t)}\bar{\rho}_{\mathrm{B}}\} = \prod_k T_k(t)$ with

$$T_k(t) = \mathrm{Tr}_k\left\{e^{2\alpha_k(t)b_k - 2\alpha_k^* b_k^\dagger}\frac{e^{-\beta\omega_k b_k^\dagger b_k}}{Z_k}\right\}$$
$$= \sum_{n=0}^{\infty}\langle n|e^{-2\alpha_k^* b_k^\dagger}e^{+2\alpha_k(t)b_k}|n\rangle e^{-2|\alpha_k(t)|^2}e^{-\beta\omega_k n}\left[1 - e^{-\beta\omega_k}\right], \quad (3.12)$$

where we have used the BCH formula (3.5) and also inserted the normalized thermal state for mode k. For the matrix element we can use the identity

$$\langle n|e^{-\sigma^* b^\dagger}e^{\sigma b}|n\rangle = \mathscr{L}_n\left(|\sigma|^2\right), \quad (3.13)$$

with the Laguerre polynomial [4]

$$\mathscr{L}_n(x) = \frac{e^x}{n!}\frac{d^n}{dx^n}\left(e^{-x}x^n\right), \quad (3.14)$$

which further yields

$$T_k(t) = \sum_{n=0}^{\infty}\mathscr{L}_n\left(4\left|\alpha_k(t)\right|^2\right)e^{-2|\alpha_k(t)|^2}e^{-\beta\omega_k n}\left[1 - e^{-\beta\omega_k}\right]$$
$$= e^{-2|\alpha_k(t)|^2\coth(\beta\omega_k/2)}. \quad (3.15)$$

Therefore, we obtain for the sought-after expectation value

$$\mathrm{Tr}_{\mathrm{B}}\left\{e^{2A(t)}\bar{\rho}_{\mathrm{B}}\right\} = e^{-2\sum_k|\alpha_k(t)|^2\coth(\beta\omega_k/2)} = \mathrm{Tr}_{\mathrm{B}}\left\{e^{-2A(t)}\bar{\rho}_{\mathrm{B}}\right\}, \quad (3.16)$$

where the second equality sign follows from $A(t) = -A^\dagger(t)$ and the fact that the above expectation value is real. The exact solution for the system density matrix becomes

$$\boldsymbol{\rho}_{\mathrm{S}}(t) = \rho_{\mathrm{S}}^0\frac{1}{2}\left[1 + e^{-2\sum_k|\alpha_k(t)|^2\coth(\beta\omega_k/2)}\right]$$
$$+ \sigma^z\rho_{\mathrm{S}}^0\sigma^z\frac{1}{2}\left[1 - e^{-2\sum_k|\alpha_k(t)|^2\coth(\beta\omega_k/2)}\right], \quad (3.17)$$

which means that, as expected, the populations ρ_{00} and ρ_{11} are unaffected by the interaction with the reservoir, whereas the coherences evolve according to

$$\boldsymbol{\rho}_{01}(t) = \rho_{01}^0 e^{-2\sum_k|\alpha_k(t)|^2\coth(\beta\omega_k/2)},$$
$$\boldsymbol{\rho}_{10}(t) = \rho_{10}^0 e^{-2\sum_k|\alpha_k(t)|^2\coth(\beta\omega_k/2)}. \quad (3.18)$$

Inserting $|\alpha_k(t)|^2 = 2\frac{|h_k|^2}{\omega_k^2}[1-\cos(\omega_k t)] = 4\frac{|h_k|^2}{\omega_k^2}\sin^2(\omega_k t/2)$, we eventually arrive at the well-known result that, in the pure dephasing model, the coherences decay as

$$\rho_{01}(t) = \exp\left\{-8\sum_k |h_k|^2 \frac{\sin^2(\omega_k t/2)}{\omega_k^2}\coth\left(\frac{\beta\omega_k}{2}\right)\right\}\rho_{01}^0, \tag{3.19}$$

which for a discrete spectrum of modes will display recurrences. Transforming to the continuum limit by introducing the spectral coupling density

$$J(\omega) = \sum_k |h_k|^2 \delta(\omega - \omega_k), \tag{3.20}$$

we note that as soon as $J(\omega)$ is represented as a smooth function, a popular choice being the parametrization [5]

$$J(\omega) = J_0 \frac{\omega^s}{\omega_{\mathrm{ph}}^{1-s}} e^{-\omega/\omega_{\mathrm{c}}}, \quad \text{for } \omega > 0, \tag{3.21}$$

the coherences will approach a vanishing stationary state $\lim_{t\to\infty} \boldsymbol{\rho}_{01}(t) = 0$.

By performing a simple time derivative of the solution, one can now derive an exact master equation. For completeness we note here that this exact master equation has time-dependent rates. In addition, it is not of Lindblad form (also for constant time) but must—since the solution is exact—nevertheless preserve positivity of the density matrix.

In general, the speed of decoherence depends on the temperature and coupling strength, etc. For high temperatures, we can expand the integrand and solve the special case $s = 1$ and $\omega_{\mathrm{c}} \to \infty$ in the above parametrization explicitly:

$$\rho_{01}(t) \approx e^{-4\pi \frac{J_0}{\beta} t} \rho_{01}^0. \tag{3.22}$$

This result can also be reproduced within a master equation approach, as described below.

3.1.3 Master Equation Approach

Identifying a single system and bath coupling operator in the interaction Hamiltonian $A = \sigma^z$ and $B = \sum_k (h_k b_k + h_k^* b_k^\dagger)$, respectively, we first calculate the bath correlation function

$$\begin{aligned} C(t) = \langle \boldsymbol{B}(t) B\rangle &= \sum_{kk'} \left\langle \left(h_k b_k e^{-\mathrm{i}\omega_k t} + h_k^* b_k^\dagger e^{+\mathrm{i}\omega_k t}\right)\left(h_{k'} b_{k'} + h_{k'}^* b_{k'}^\dagger\right)\right\rangle \\ &= \sum_k |h_k|^2 \left\{e^{-\mathrm{i}\omega_k t}\left[1 + n_B(\omega_k)\right] + e^{+\mathrm{i}\omega_k t} n_B(\omega_k)\right\} \end{aligned}$$

$$
\begin{aligned}
&= \int_0^{\infty} J(\omega)\left\{e^{-\mathrm{i}\omega t}\left[1+n_B(\omega)\right]+e^{+\mathrm{i}\omega t}n_B(\omega)\right\}d\omega \\
&= \int_{-\infty}^{+\infty} J(\omega)e^{-\mathrm{i}\omega t}J(\omega)\left[1+n_B(\omega)\right]d\omega,
\end{aligned}
\tag{3.23}
$$

where we have analytically continued the spectral coupling density to negative frequencies $J(-\omega)=-J(\omega)$. This enables us to identify the Fourier transform of the correlation function as

$$
\gamma(\omega)=2\pi J(\omega)\left[1+n_B(\omega)\right]. \tag{3.24}
$$

With the help of Eq. (2.38) this can be used to calculate the odd Fourier transform numerically. The quantum optical master equation in Definition 2.3 then yields

$$
\begin{aligned}
\dot{\rho}_{00} &= \dot{\rho}_{11}=0, \\
\dot{\rho}_{01} &= -\mathrm{i}(E_0-E_1+\sigma_{00}-\sigma_{11})\rho_{01}+\left(\gamma_{00,11}-\frac{1}{2}\gamma_{00,00}-\frac{1}{2}\gamma_{11,11}\right)\rho_{01} \\
&= -\mathrm{i}(E_0-E_1+\sigma_{00}-\sigma_{11})\rho_{01}-2\gamma(0)\rho_{01}.
\end{aligned}
\tag{3.25}
$$

The first two equations just express the fact that the interaction does not change the system energy, which is also obeyed by the master equation solution.

The Lamb-shift terms can be expressed with the odd Fourier transform of the reservoir correlation function $\sigma_{00}=\sigma(0)/(2\mathrm{i})=\sigma_{11}$, and thus they cancel in the evolution of the coherences. Therefore, we obtain for the coherences a decay according to $\rho_{01}(t)=e^{-\mathrm{i}(E_0-E_1)t}e^{-2\gamma(0)t}|\rho_{01}^0|$. The first exponential can be transformed away by switching to the interaction picture $\boldsymbol{\rho}_{\mathrm{S}}(t)=e^{+\mathrm{i}H_{\mathrm{S}}t}\rho_{\mathrm{S}}(t)e^{-\mathrm{i}H_{\mathrm{S}}t}$, where one only has $\boldsymbol{\rho}_{01}(t)=e^{-2\gamma(0)t}|\rho_{01}^0|$. Now, assuming high temperatures and an ohmic spectral coupling density $J(\omega)=J_0\omega$, the limit becomes $\lim_{\omega\to 0}\gamma(0)=2\pi J_0/\beta$, which perfectly coincides with the result in Eq. (3.22).

We finally note that the Lindblad form only guarantees positivity of the solution if initialized with a valid, i.e., positive, density matrix.

3.2 Quantum Dot Coupled to Two Fermionic Leads

As one of the simplest fermionic models, we consider a single electron transistor (SET). The system, bath, and interaction Hamiltonians are given by

$$
\begin{aligned}
H_{\mathrm{S}} &= \varepsilon d^\dagger d, \qquad H_{\mathrm{B}}=\sum_k \varepsilon_{kL}c_{kL}^\dagger c_{kL}+\sum_k \varepsilon_{kR}c_{kR}^\dagger c_{kR}, \\
H_{\mathrm{I}} &= \sum_k\left(t_{kL}dc_{kL}^\dagger+t_{kL}^*c_{kL}d^\dagger\right)+\sum_k\left(t_{kR}dc_{kR}^\dagger+t_{kR}^*c_{kR}d^\dagger\right),
\end{aligned}
\tag{3.26}
$$

where d is a fermionic annihilation operator on the dot and $c_{k\alpha}$ are fermionic annihilation operators of an electron in the kth mode of lead α. Obviously, this corresponds to a quadratic fermionic Hamiltonian, which can in principle be solved exactly by various methods, such as non-equilibrium Green's functions [6] or even the equation of motion approach [7]. Such quadratic models are useful for studying exact transport properties [8] or exact master equations [9].

3.2.1 Heisenberg Picture Dynamics

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

$$\begin{aligned} \dot{\boldsymbol{d}} &= -\mathrm{i}\varepsilon \boldsymbol{d} + \mathrm{i}\sum_k \left[t_{kL}^* \boldsymbol{c}_{kL} + t_{kR}^* \boldsymbol{c}_{kR}\right], \\ \dot{\boldsymbol{c}}_{kL} &= -\mathrm{i}\varepsilon_{kL} \boldsymbol{c}_{kL} + \mathrm{i} t_{kL} \boldsymbol{d}, \\ \dot{\boldsymbol{c}}_{kR} &= -\mathrm{i}\varepsilon_{kR} \boldsymbol{c}_{kR} + \mathrm{i} t_{kR} \boldsymbol{d}. \end{aligned} \tag{3.27}$$

Surprisingly, this system is already closed, and we obtain its solution by performing a Laplace transform [10]:

$$\begin{aligned} z\tilde{d}(z) - d &= -\mathrm{i}\varepsilon \tilde{d}(z) + \mathrm{i}\sum_k \left[t_{kL}^* \tilde{c}_{kL}(z) + t_{kR}^* \tilde{c}_{kR}(z)\right], \\ z\tilde{c}_{kL}(z) - c_{kL} &= -\mathrm{i}\varepsilon_{kL}\tilde{c}_{kL}(z) + \mathrm{i} t_{kL}\tilde{d}(z), \\ z\tilde{c}_{kR}(z) - c_{kR} &= -\mathrm{i}\varepsilon_{kR}\tilde{c}_{kR}(z) + \mathrm{i} t_{kR}\tilde{d}(z). \end{aligned} \tag{3.28}$$

In the above equations, we can eliminate the operators $\tilde{c}_{kL}(z)$ and $\tilde{c}_{kR}(z)$. This yields for the dot annihilation operator

$$\begin{aligned} \tilde{d}(z) &= \frac{d + \mathrm{i}\sum_k \left(\frac{t_{kL}^* c_{kL}}{z+\mathrm{i}\varepsilon_{kL}} + \frac{t_{kR}^* c_{kR}}{z+\mathrm{i}\varepsilon_{kR}}\right)}{z + \mathrm{i}\varepsilon + \sum_k \left(\frac{|t_{kL}|^2}{z+\mathrm{i}\varepsilon_{kL}} + \frac{|t_{kR}|^2}{z+\mathrm{i}\varepsilon_{kR}}\right)} \\ &\equiv \tilde{f}(z) d + \sum_k \left(\tilde{g}_{kL}(z) c_{kL} + \tilde{g}_{kR}(z) c_{kR}\right), \end{aligned} \tag{3.29}$$

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

$$\tilde{c}_{k\alpha}(z) = \frac{1}{z + \mathrm{i}\varepsilon_{k\alpha}} c_{k\alpha} + \frac{\mathrm{i} t_{k\alpha}}{z + \mathrm{i}\varepsilon_{k\alpha}} \tilde{d}(z). \tag{3.30}$$

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.

3.2.2 Stationary Occupation

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

$$
\begin{aligned}
n(t) &= \left\langle \left[f^*(t)d^\dagger + \sum_k \left(g^*_{kL}(t)c^\dagger_{kL} + g^*_{kR}(t)c^\dagger_{kR} \right) \right] \right. \\
&\quad \times \left. \left[f(t)d + \sum_k \left(g_{kL}(t)c_{kL} + g_{kR}(t)c_{kR} \right) \right] \right\rangle \\
&= \left| f(t) \right|^2 n_0 + \sum_k \left(\left| g_{kL}(t) \right|^2 f_L(\varepsilon_{kL}) + \left| g_{kR}(t) \right|^2 f_R(\varepsilon_{kR}) \right),
\end{aligned}
\tag{3.31}
$$

where we have used a product state as an initial one,

$$
\rho_0 = \rho^0_{\mathrm{S}} \frac{e^{-\beta_L(H_L - \mu_L N_L)}}{Z_L} \frac{e^{-\beta_R(H_R - \mu_R N_R)}}{Z_R}
\tag{3.32}
$$

with the lead Hamiltonians $H_\alpha = \sum_k \varepsilon_{k\alpha} c^\dagger_{k\alpha} c_{k\alpha}$ and the lead particle numbers $N_\alpha = \sum_k c^\dagger_{k\alpha} c_{k\alpha}$. These eventually yield the only nonvanishing expectation values $n_0 = \langle d^\dagger d\rangle$ and $f_\alpha(\varepsilon_{k\alpha}) = \langle c^\dagger_{k\alpha} c_{k\alpha}\rangle$. Inverse lead temperatures β_α and chemical potentials μ_α thereby only enter implicitly in the Fermi functions. Therefore, to find the exact solution for the time-dependent dot occupation, we have to find the inverse Laplace transform of the following:

$$
\begin{aligned}
\tilde{f}(z) &= \frac{1}{z + \mathrm{i}\varepsilon + \sum_k \left(\frac{|t_{kL}|^2}{z + \mathrm{i}\varepsilon_{kL}} + \frac{|t_{kR}|^2}{z + \mathrm{i}\varepsilon_{kR}} \right)}, \\
\tilde{g}_{k\alpha}(z) &= \frac{\mathrm{i}t^*_{k\alpha}}{[z + \mathrm{i}\varepsilon_{k\alpha}][z + \mathrm{i}\varepsilon + \sum_k \left(\frac{|t_{kL}|^2}{z + \mathrm{i}\varepsilon_{kL}} + \frac{|t_{kR}|^2}{z + \mathrm{i}\varepsilon_{kR}} \right)]},
\end{aligned}
\tag{3.33}
$$

which heavily depends on the number of modes and their distribution in the reservoir. For example, any system with a finite number of reservoir modes 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, for simplicity we assume $N + 1$ modes in each reservoir, $-N/2 \leq k \leq +N/2$. These are distributed over the energies as $\varepsilon_{k\alpha} = k\Omega/\sqrt{N}$ and are assumed to couple more weakly to the dot as their momentum increases:

$$|t_{k\alpha}|^2 = \frac{\Omega}{2\pi\sqrt{N}} \frac{\Gamma_\alpha \delta_\alpha^2}{(k\Omega/\sqrt{N})^2 + \delta_\alpha^2}. \tag{3.34}$$

Letting the number of reservoir modes N go to infinity, we can replace the summation in the denominators by a continuous integral:

$$\begin{aligned}
\tilde{f}(z) &\approx \frac{1}{z + \mathrm{i}\varepsilon + \int \frac{1}{2\pi}\left(\frac{\Gamma_L\delta_L^2}{\omega^2+\delta_L^2} + \frac{\Gamma_R\delta_R^2}{\omega^2+\delta_R^2}\right)\frac{1}{z+\mathrm{i}\omega}\,d\omega} = \frac{1}{z + \mathrm{i}\varepsilon + \frac{1}{2}\left(\frac{\Gamma_L\delta_L}{z+\delta_L} + \frac{\Gamma_R\delta_R}{z+\delta_R}\right)}, \\
\tilde{g}_{k\alpha}(z) &\approx \frac{\mathrm{i}t_{k\alpha}^*}{(z+\mathrm{i}\varepsilon_{k\alpha})[z + \mathrm{i}\varepsilon + \int \frac{1}{2\pi}\left(\frac{\Gamma_L\delta_L^2}{\omega^2+\delta_L^2} + \frac{\Gamma_R\delta_R^2}{\omega^2+\delta_R^2}\right)\frac{1}{z+\mathrm{i}\omega}\,d\omega]} \\
&= \frac{1}{[z+\mathrm{i}\varepsilon_{k\alpha}][z + \mathrm{i}\varepsilon + \frac{1}{2}\left(\frac{\Gamma_L\delta_L}{z+\delta_L} + \frac{\Gamma_R\delta_R}{z+\delta_R}\right)]}.
\end{aligned} \tag{3.35}$$

We note that this transfer from a discrete to a continuous spectrum of reservoir modes is commonly performed formally by introducing the energy-dependent tunneling rates

$$\Gamma_\alpha(\omega) = 2\pi \sum_k |t_{k\alpha}|^2 \delta(\omega - \varepsilon_{k\alpha}). \tag{3.36}$$

Here, we have thereby assumed a Lorentzian-shaped tunneling rate [11]

$$\Gamma_\alpha(\omega) = \frac{\Gamma_\alpha \delta_\alpha^2}{\omega^2 + \delta_\alpha^2}. \tag{3.37}$$

The simple pole structure of these tunneling rates renders analytic calculations simple. Superpositions of many Lorentzian shapes with shifted centers may approximate quite general tunneling rates [12].

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

$$\begin{aligned}
\tilde{f}(z) &\to \frac{1}{z + \mathrm{i}\varepsilon + (\Gamma_L + \Gamma_R)/2}, \\
\tilde{g}_{k\alpha}(z) &\to \frac{\mathrm{i}t_{k\alpha}^*}{(z+\mathrm{i}\varepsilon_{k\alpha})[z + \mathrm{i}\varepsilon + (\Gamma_L + \Gamma_R)/2]}.
\end{aligned} \tag{3.38}$$

Inserting the inverse Laplace transforms of these expressions,

$$
\begin{aligned}
f(t) &\to e^{-i\varepsilon t} e^{-\Gamma t/2}, \\
g_{k\alpha}(t) &\to \frac{t_{k\alpha}^*(e^{-i\varepsilon t} e^{-\Gamma t/2} - e^{-i\varepsilon_{k\alpha} t})}{\varepsilon_{k\alpha} - \varepsilon + i\Gamma/2}
\end{aligned}
\tag{3.39}
$$

(with $\Gamma \equiv \Gamma_L + \Gamma_R$) into Eq. (3.31), we obtain by switching to a continuum representation

$$
\begin{aligned}
n(t) &= e^{-\Gamma t} n_0 + \sum_k \sum_\alpha |t_{k\alpha}|^2 f_\alpha(\varepsilon_{k\alpha}) 4 \frac{1 - 2e^{-\Gamma t/2} \cos[(\varepsilon_{k\alpha} - \varepsilon)t] + e^{-\Gamma t}}{\Gamma^2 + 4(\varepsilon_{k\alpha} - \varepsilon)^2} \\
&= e^{-\Gamma t} n_0 + \sum_\alpha \int d\omega \Gamma_\alpha f_\alpha(\omega) \frac{4}{2\pi} \frac{1 - 2e^{-\Gamma t/2} \cos[(\omega - \varepsilon)t] + e^{-\Gamma t}}{\Gamma^2 + 4(\omega - \varepsilon)^2}.
\end{aligned}
\tag{3.40}
$$

The long-term limit can, because $\Gamma \geq 0$, be read off easily, and the stationary occupation becomes

$$
\bar{n} = \sum_\alpha \int d\omega\, \Gamma_\alpha f_\alpha(\omega) \frac{2}{\pi} \frac{1}{\Gamma^2 + 4(\omega - \varepsilon)^2}. \tag{3.41}
$$

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., $\bar{n} = f_L(\varepsilon) + \mathscr{O}\{\Gamma_L\}$). 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

$$
\bar{n} \to \frac{\Gamma_L f_L(\varepsilon) + \Gamma_R f_R(\varepsilon)}{\Gamma_L + \Gamma_R}, \tag{3.42}
$$

which is also obtained within a master equation approach (compare Sect. 5.1).

Exercise 3.4 (Weak coupling limit) Show that Eq. (3.41) reduces in the weak-coupling limit to Eq. (3.42) by using a representation of the Dirac delta distribution,

$$
\delta(x) = \lim_{\varepsilon \to 0} \frac{1}{\pi} \frac{\varepsilon}{x^2 + \varepsilon^2}.
$$

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.

3.2.3 Stationary Current

The stationary current from left to right through the SET can be defined as the long-term limit of the change of particle numbers at the right lead,

$$I = \lim_{t\to\infty} \frac{d}{dt}\left\langle \sum_k c_{kR}^\dagger c_{kR} \right\rangle, \tag{3.43}$$

which we can evaluate in the Heisenberg picture as we did for the stationary occupation. Using Eq. (3.30), the right lead modes can be written as

$$\begin{aligned}\tilde{c}_{kR}(z) &= \frac{\mathrm{i}t_{kR}}{(z+\mathrm{i}\varepsilon_{kR})(z+\mathrm{i}\varepsilon+\Gamma/2)} d + \frac{1}{z+\mathrm{i}\varepsilon_{kR}} c_{kR} \\ &\quad - \sum_q \frac{t_{kR}t_{qL}^*}{(z+\mathrm{i}\varepsilon_{kR})(z+\mathrm{i}\varepsilon_{qL})(z+\mathrm{i}\varepsilon+\Gamma/2)} c_{qL} \\ &\quad - \sum_q \frac{t_{kR}t_{qR}^*}{(z+\mathrm{i}\varepsilon_{kR})(z+\mathrm{i}\varepsilon_{qR})(z+\mathrm{i}\varepsilon+\Gamma/2)} c_{qR}.\end{aligned} \tag{3.44}$$

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

$$\begin{aligned}\boldsymbol{c}_{kR}(t) &\to \left(-\frac{t_{kR}e^{-\mathrm{i}\varepsilon_{kR}t}}{\varepsilon_{kR}-\varepsilon+\mathrm{i}\Gamma/2}\right) d + e^{-\mathrm{i}\varepsilon_{kR}t} c_{kR} \\ &\quad + \sum_q \frac{t_{kR}t_{qL}^*}{\varepsilon_{kR}-\varepsilon_{qL}} \left(\frac{e^{-\mathrm{i}\varepsilon_{qL}t}}{\varepsilon_{qL}-\varepsilon+\mathrm{i}\Gamma/2} - \frac{e^{-\mathrm{i}\varepsilon_{kR}t}}{\varepsilon_{kR}-\varepsilon+\mathrm{i}\Gamma/2}\right) c_{qL} \\ &\quad + \sum_q \frac{t_{kR}t_{qR}^*}{\varepsilon_{kR}-\varepsilon_{qR}} \left(\frac{e^{-\mathrm{i}\varepsilon_{qR}t}}{\varepsilon_{qR}-\varepsilon+\mathrm{i}\Gamma/2} - \frac{e^{-\mathrm{i}\varepsilon_{kR}t}}{\varepsilon_{kR}-\varepsilon+\mathrm{i}\Gamma/2}\right) c_{qR}.\end{aligned} \tag{3.45}$$

The occupation of the right lead therefore becomes

$$\begin{aligned}N_R &\to \sum_k \frac{|t_{kR}|^2}{(\varepsilon_{kR}-\varepsilon)^2+\Gamma^2/4} n_0 + N_R^0 \\ &\quad - \sum_{kq} \left[\frac{t_{kR}t_{qR}^*}{\varepsilon_{kR}-\varepsilon_{qR}} e^{+\mathrm{i}\varepsilon_{kR}t} \right.\end{aligned}$$

$$\times\left(\frac{e^{-\mathrm{i}\varepsilon_{qR}t}}{\varepsilon_{qR}-\varepsilon+\mathrm{i}\Gamma/2}-\frac{e^{-\mathrm{i}\varepsilon_{kR}t}}{\varepsilon_{kR}-\varepsilon+\mathrm{i}\Gamma/2}\right)\delta_{kq}f_R(\varepsilon_{kR})+\text{h.c.}\Bigg]$$

$$+\sum_{kq}\frac{|t_{kR}|^2|t_{qL}|^2}{(\varepsilon_{kR}-\varepsilon_{qL})^2}\left(\frac{e^{+\mathrm{i}\varepsilon_{qL}t}}{\varepsilon_{qL}-\varepsilon-\mathrm{i}\Gamma/2}-\frac{e^{+\mathrm{i}\varepsilon_{kR}t}}{\varepsilon_{kR}-\varepsilon-\mathrm{i}\Gamma/2}\right)$$

$$\times\left(\frac{e^{-\mathrm{i}\varepsilon_{qL}t}}{\varepsilon_{qL}-\varepsilon+\mathrm{i}\Gamma/2}-\frac{e^{-\mathrm{i}\varepsilon_{kR}t}}{\varepsilon_{kR}-\varepsilon+\mathrm{i}\Gamma/2}\right)f_L(\varepsilon_{qL})$$

$$+\sum_{kq}\frac{|t_{kR}|^2|t_{qR}|^2}{(\varepsilon_{kR}-\varepsilon_{qR})^2}\left(\frac{e^{+\mathrm{i}\varepsilon_{qR}t}}{\varepsilon_{qR}-\varepsilon-\mathrm{i}\Gamma/2}-\frac{e^{+\mathrm{i}\varepsilon_{kR}t}}{\varepsilon_{kR}-\varepsilon-\mathrm{i}\Gamma/2}\right)$$

$$\times\left(\frac{e^{-\mathrm{i}\varepsilon_{qR}t}}{\varepsilon_{qR}-\varepsilon+\mathrm{i}\Gamma/2}-\frac{e^{-\mathrm{i}\varepsilon_{kR}t}}{\varepsilon_{kR}-\varepsilon+\mathrm{i}\Gamma/2}\right)f_R(\varepsilon_{qR}). \tag{3.46}$$

The first term is just triggered by the initial occupation of the dot, and the second term corresponds to the initial occupation of the right lead. These terms are constant and cannot contribute to the current, which however is different for all other terms. Introducing the tunneling rates in the wide-band limit $\Gamma_\alpha \approx \Gamma_\alpha(\omega) = \sum_k |t_{k\alpha}|^2\delta(\omega-\varepsilon_{k\alpha})$, we can represent the right lead occupation by integrals:

$$\begin{aligned}
N_R \to{}& \frac{1}{2\pi}\int d\omega\,\frac{\Gamma_R}{(\omega-\varepsilon)^2+\Gamma^2/4}n_0\\
&+N_R^0-\frac{1}{2\pi}\int d\omega\,\Gamma_R f_R(\omega)\left[\frac{4+4\mathrm{i}\omega t-2t(\Gamma+2\mathrm{i}\varepsilon)}{(2\omega+\mathrm{i}\Gamma-2\varepsilon)^2}+\text{h.c.}\right]\\
&+\frac{1}{4\pi^2}\int d\omega\,d\omega'\big(\Gamma_L\Gamma_R f_L(\omega')+\Gamma_R^2 f_R(\omega')\big)\frac{1}{(\omega-\omega')^2}\\
&\times\left|\frac{e^{-\mathrm{i}\omega' t}}{\omega'-\varepsilon+\mathrm{i}\Gamma/2}-\frac{e^{-\mathrm{i}\omega t}}{\omega-\varepsilon+\mathrm{i}\Gamma/2}\right|^2.
\end{aligned}\tag{3.47}$$

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

$$\begin{aligned}
F(\omega') \equiv{}& \lim_{t\to\infty}\frac{d}{dt}\int d\omega\,\frac{1}{(\omega-\omega')^2}\left|\frac{e^{-\mathrm{i}\omega' t}}{\omega'-\varepsilon+\mathrm{i}\Gamma/2}-\frac{e^{-\mathrm{i}\omega t}}{\omega-\varepsilon+\mathrm{i}\Gamma/2}\right|^2\\
={}& \lim_{z\to 0} z\int_0^\infty dt\, e^{-zt}\,\frac{d}{dt}\int d\omega\frac{1}{(\omega-\omega')^2}\left|\frac{e^{-\mathrm{i}\omega' t}}{\omega'-\varepsilon+\mathrm{i}\Gamma/2}-\frac{e^{-\mathrm{i}\omega t}}{\omega-\varepsilon+\mathrm{i}\Gamma/2}\right|^2\\
={}& \frac{8\pi}{\Gamma^2+4(\omega'-\varepsilon)^2},
\end{aligned}\tag{3.48}$$

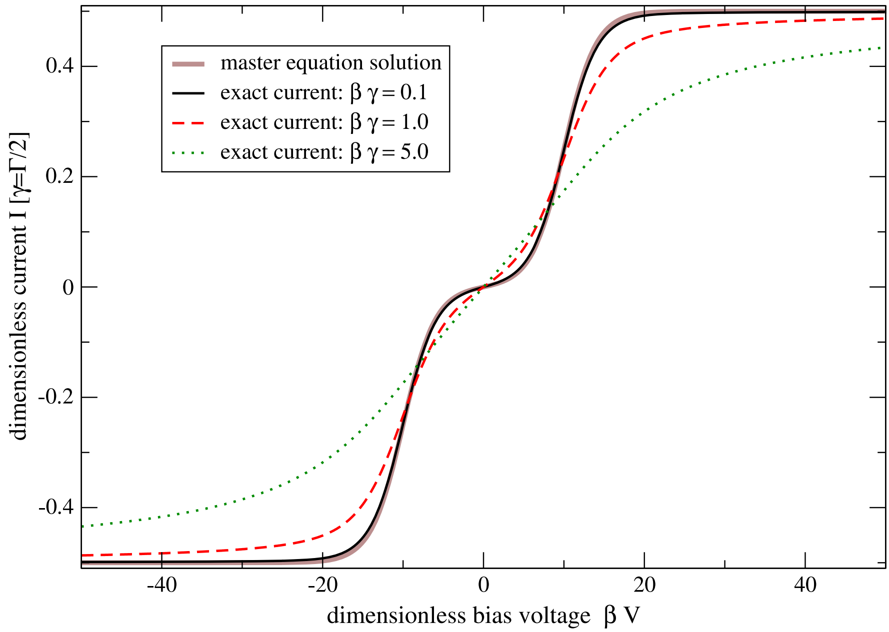

Fig. 3.1 Plot of the electronic matter current (in units of $\gamma = \Gamma_L = \Gamma_R = \Gamma/2$) versus the bias voltage for symmetric tunneling rates and equal electronic temperatures $\beta_L = \beta_R = \beta$ and dot level $\beta\varepsilon = 5$. For a small coupling strength, the exact (*black solid*) and master equation (*brown bold*) solutions coincide for all bias voltages. For stronger couplings (*red dashed* and *green dotted*, respectively), the determination of the dot level ε from steps in the current is no longer possible (Color figure online)

which with its Lorentzian shape converges for small Γ towards a Dirac delta distribution. The current becomes

$$\begin{aligned} I &= -\frac{1}{\pi}\int d\omega\, \Gamma_R f_R(\omega) \frac{\Gamma/2}{(\omega-\varepsilon)^2 + (\Gamma/2)^2} \\ &\quad + \frac{1}{\pi\Gamma}\int d\omega \big(\Gamma_L\Gamma_R f_L(\omega) + \Gamma_R^2 f_R(\omega)\big) \frac{\Gamma/2}{(\omega-\varepsilon)^2 + (\Gamma/2)^2} \\ &= \frac{\Gamma_L\Gamma_R}{\Gamma_L+\Gamma_R}\int d\omega \big[f_L(\omega) - f_R(\omega)\big] \frac{1}{\pi}\frac{\Gamma/2}{(\omega-\varepsilon)^2 + (\Gamma/2)^2}. \end{aligned} \tag{3.49}$$

Alternatively, this expression can also be derived by evaluating the expectation value of the current operator directly $I = \mathrm{i}\sum_k t_{kR}\langle \boldsymbol{c}_{kR}^\dagger(t)\boldsymbol{d}(t)\rangle + \text{h.c.}$ 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 Green's functions [6]. For consistency, we note that the current is antisymmetric under the exchange of left and right leads as expected.

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

$$I = \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} \left[f_L(\varepsilon) - f_R(\varepsilon) \right], \tag{3.50}$$

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.

Exercise 3.5 (Weak coupling limit) Show that Eq. (3.50) follows from Eq. (3.49) when $\Gamma \to 0$.

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 with Eq. (3.50). In Sect. 5.1 we will find that the master equation approach applied to the same problem reproduces Eq. (3.50) and therefore coincides with the exact result in the infinite bias limit.

Figure 3.1 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 example shown, spectroscopy of the dot level ε via detecting steps in the I–V characteristics is therefore only possible in the weak coupling limit.

References

1. W.G. Unruh, Maintaining coherence in quantum computers. Phys. Rev. A **51**, 992 (1995)
2. J.H. Reina, L. Quiroga, N.F. Johnson, Decoherence of quantum registers. Phys. Rev. A **65**, 032326 (2002)
3. D.A. Lidar, Z. Bihary, K.B. Whaley, From completely positive maps to the quantum Markovian semigroup master equation. Chem. Phys. **268**, 35 (2001)
4. M. Abramowitz, I.A. Stegun (eds.), Handbook of Mathematical Functions (National Bureau of Standards, 1970)
5. T. Brandes, Coherent and collective quantum optical effects in mesoscopic systems. Phys. Rep. **408**, 315 (2005)
6. H. Haug, A.-P. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors* (Springer, Berlin, 2008)
7. G. Schaller, P. Zedler, T. Brandes, Systematic perturbation theory for dynamical coarse-graining. Phys. Rev. A **79**, 032110 (2009)
8. A. Dhar, K. Saito, P. Hänggi, Nonequilibrium density-matrix description of steady-state quantum transport. Phys. Rev. E **85**, 011126 (2012)
9. L.-P. Yang, C.Y. Cai, D.Z. Xu, W.-M. Zhang, C.P. Sun, Master equation and dispersive probing of a non-Markovian process. Phys. Rev. A **87**, 012110 (2013)
10. G.B. Arfken, H.J. Weber, *Mathematical Methods for Physicists* (Elsevier, Oxford, 2005)
11. P. Zedler, G. Schaller, G. Kießlich, C. Emary, T. Brandes, Weak coupling approximations in non-Markovian transport. Phys. Rev. B **80**, 045309 (2009)
12. U. Kleinekathöfer, Non-Markovian theories based on a decomposition of the spectral density. J. Chem. Phys. **121**, 2505 (2004)