Open quantum systems – lecture 8

lecture
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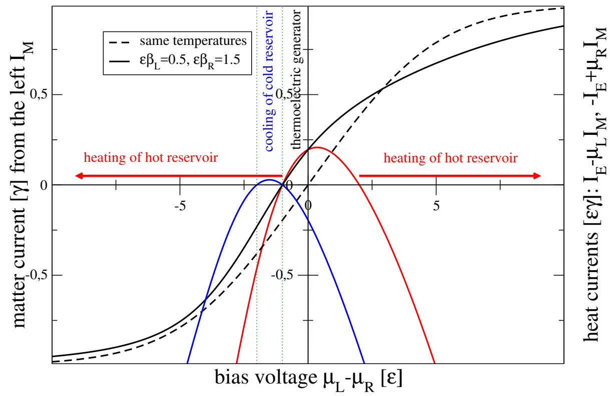

Figure 2.1: Plot of the matter current $\bar{I}_M$ (solid black) and heat currents entering from left ($\dot{\bar{Q}}^{(L)}$, solid red) and right ($\dot{\bar{Q}}^{(R)}$, solid blue) versus bias voltage. The dashed reference is temperatures $\epsilon\beta_\alpha = 1$. For large bias voltages, both reservoirs are heated (conventional heater). There is a region where $-\bar{I}_M(\mu_L - \mu_R) > 0$, where the system acts as thermoelectric generator, and to the left of it there is a region where the cold right reservoir is cooled while simultaneously the hot left reservoir is heated (blue text). Here, the system acts as a true heat pump.

2.5 Quantum transport in rate equations

2.5.1 Example: The single-electron transistor

For the previously discussed example of the single-electron transistor with two reservoirs it is straightforward to show that the dynamics of the populations $(P_0, P_1) = (\rho_{00}, \rho_{11})$ follows a simple rate equation, additive in the reservoirs

$$\mathcal{L} = \begin{pmatrix} -\Gamma_L f_L - \Gamma_R f_R & +\Gamma_L(1-f_L) + \Gamma_R(1-f_R) \\ +\Gamma_L f_L + \Gamma_R f_R & -\Gamma_L(1-f_L) - \Gamma_R(1-f_R) \end{pmatrix} . \tag{2.1}$$

This implies for the currents from left to right

$$\bar{I}_M = \bar{I}_M^{(L)} = \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R}(f_L - f_R) , \qquad \bar{I}_E = \bar{I}_E^{(L)} = \epsilon \bar{I}_M , \tag{2.2}$$

where ϵ denotes the dot level, at which the Fermi functions and tunneling rates are evaluated

$$f_\nu = \frac{1}{e^{\beta_\nu(\epsilon - \mu_\nu)} + 1} , \qquad \Gamma_\nu = \Gamma_\nu(\epsilon) = 2\pi \sum_k |t_{k\nu}|^2 \delta(\epsilon - \epsilon_{k\nu}) . \tag{2.3}$$

We can plot the currents versus the bias voltage at $\mu_L = +V/2$ and $\mu_R = -V/2$ to identify the regimes where the device acts as thermoelectric generator or refrigerator, see Fig. 2.1. Furthermore, we can easily calculate the currents from left to right explicitly

$$I_M = \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R}[f_L - f_R] , \qquad I_E = \epsilon I_M . \tag{2.4}$$

At sufficiently low temperatures, this will show for $\mu_L = V/2 = -\mu_R$ a step at bias voltage $V = \pm 2\epsilon$ from vanishing current to the infinite bias limit $\pm\frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R}$.

2.5.2 Example: The double quantum dot

For the double quantum dot, described by the system Hamiltonian (that the on-site energies are identical is just for simplicity)

$$H_S = \epsilon(d_L^\dagger d_L + d_R^\dagger d_R) + T(d_L^\dagger d_R + d_R^\dagger d_L) + U d_L^\dagger d_L d_R^\dagger d_R \tag{2.5}$$

one can find a simple transformation to new fermionic operators that diagonalizes the system Hamiltonian while preserving the fermionic anticommutation relations

$$d_L = \frac{1}{\sqrt{2}}(d_+ + d_-)\,, \qquad d_R = \frac{1}{\sqrt{2}}(d_+ - d_-)\,. \tag{2.6}$$

Written in terms of the new fermionic operators, the system Hamiltonian becomes

$$H_S = (\epsilon + T)d_+^\dagger d_+ + (\epsilon - T)d_-^\dagger d_- + U d_+^\dagger d_+ d_-^\dagger d_-\,, \tag{2.7}$$

which has the advantage of being diagonal in the Fock basis.

Superpositions of states with different total charge cannot be created, such that only two valid coherences are allowed. In a master equation, the others are formally still there but will decouple from the populations and can be omitted to reduce the dimension of the problem. Thus, vectorizing the relevant density matrix elements populations as $(\rho_{00}, \rho_{--}, \rho_{++}, \rho_{22}, \rho_{-+}, \rho_{+-})^{\mathrm{T}}$, the Lindbladian thus assumes the form

$$\mathcal{L} = \begin{pmatrix} \mathcal{L}_{\mathrm{pop}} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \kappa & 0 \\ \mathbf{0} & 0 & \kappa^* \end{pmatrix}\,, \tag{2.8}$$

where $\mathcal{L}_{\mathrm{pop}} = \mathcal{L}_{\mathrm{pop}}^L + \mathcal{L}_{\mathrm{pop}}^R$ is a 4×4 rate matrix acting only on the populations (Pauli rate equation), and κ with $\Re(\kappa) > 0$ describes the decay of coherences. Assuming the spectral densities to be constant, the rate matrices become

$$\mathcal{L}_{\mathrm{pop}}^\nu = \frac{\Gamma_\nu}{2}\begin{pmatrix} -[\ldots] & 1 - f_\nu(\epsilon - T) & 1 - f_\nu(\epsilon + T) & 0 \\ f_\nu(\epsilon - T) & -[\ldots] & 0 & 1 - f_\nu(\epsilon + T + U) \\ f_\nu(\epsilon + T) & 0 & -[\ldots] & 1 - f_\nu(\epsilon - T + U) \\ 0 & f_\nu(\epsilon + T + U) & f_\nu(\epsilon - T + U) & -[\ldots] \end{pmatrix}\,, \tag{2.9}$$

where the diagonals are fixed by demanding that the column sums of every column must vanish. The prefactor of 1/2 emerges as the system coupling operator matrix elements are evaluated in the energy eigenbasis.

This matrix can be further simplified in special cases.

For example, considering the infinite bias limits $f_L(\Delta E) \to 1$ and $f_R(\Delta E) \to 0$, the rate matrices become

$$\mathcal{L}_{\mathrm{pop}}^L \to \frac{\Gamma_L}{2}\begin{pmatrix} -2 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix}\,, \qquad \mathcal{L}_{\mathrm{pop}}^R = \frac{\Gamma_R}{2}\begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & -2 \end{pmatrix}\,, \tag{2.10}$$

which shows that the left reservoir will in this case always fill the system whereas the right reservoir will always deplete it. Simple analytic formulas can be obtained for the stationary currents in this case.

Another relevant limit is the Coulomb-blockade limit where the Coulomb interaction U is so large that the corresponding Fermi functions vanish $f_\nu(\Delta E + U) \to 0$, which yields

$$\mathcal{L}_{\mathrm{pop}}^\nu \to \frac{\Gamma_\nu}{2}\begin{pmatrix} -[\ldots] & 1 - f_\nu(\epsilon - T) & 1 - f_\nu(\epsilon + T) & 0 \\ f_\nu(\epsilon - T) & -[\ldots] & 0 & 1 \\ f_\nu(\epsilon + T) & 0 & -[\ldots] & 1 \\ 0 & 0 & 0 & -2 \end{pmatrix}\,, \tag{2.11}$$

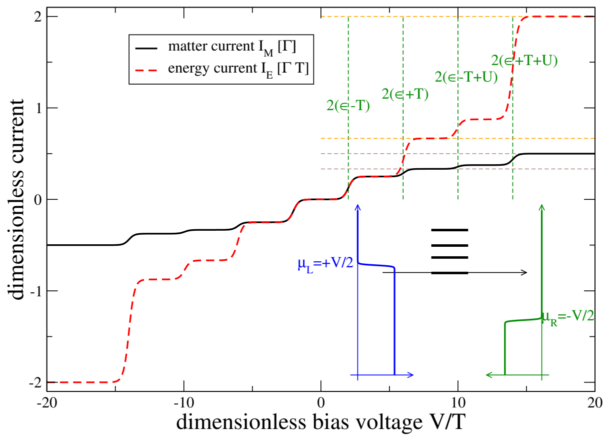

Figure 2.2: Plot of stationary matter (solid black) and energy (dashed red) currents through the DQD. The steps (vertical dashed lines) occur for positive bias voltage at $\mu_L = V/2 \in \{\epsilon - T, \epsilon + T, \epsilon - T + U, \epsilon + T + U\}$. Horizontal dashed lines mark the infinite-bias and Coulomb-blockade high-bias regimes. Other parameters have been chosen as $\mu_L = -\mu_R = V/2$, $\Gamma_L = \Gamma_R = \Gamma$, $\epsilon = 2T$, $U = 4T$, and $\beta T = 10$.

which shows that the doubly occupied state can only decay but never be populated. Thus, for steady-state considerations, it may be completely omitted and we can proceed with the remaining 3×3 submatrix describing the dynamics of ρ_{00}, ρ_{--}, and ρ_{++}. Also the remaining submatrix can be simplified further by considering a Coulomb-blockade-high-bias limit

$$\mathcal{L}^L_{\rm pop} \to \frac{\Gamma_L}{2}\begin{pmatrix} -2 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \qquad \mathcal{L}^R_{\rm pop} = \frac{\Gamma_R}{2}\begin{pmatrix} 0 & 1 & 1 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{2.12}$$

We see that these simplified rate matrices do no longer depend on T, they would thus yield finite currents even in the limit $T \to 0$, where we have a disconnected structure. This unphysical result results from the fact that the secular approximation (which we used in deriving the rate equation) is then no longer valid, as the splitting between $E_\pm = \epsilon \pm T$ vanishes. Thus, when using plug-and-play master equations like the Born-Markov-secular one, it is necessary to mind the regimes of validity.

At finite bias voltages, it becomes of course harder to calculate steady states and stationary currents. However, for low temperatures, the Fermi functions will behave similar to step functions, and the transport window becomes sharp. Then, by enlarging the bias voltage, the transport window is opened, and the currents will exhibit steps when a new transport channel is inside the transport window, see Fig. 2.2. There, one observes that the plateaus can be understood by investigating previously discussed limits (horizontal dashed curves), that occur at the predicted steps when a transition energy enters the transport window. A further obvious observation is that at zero bias voltage, we have vanishing currents. This must happen at equal temperatures. The entropy production in this case is fully determined by the matter current $\dot{S}_{\rm i} = \beta(\mu_L - \mu_R)\bar{I}_M$, where $\bar{I}_M$ denotes the current from left to right. Identifying $P_{\rm diss} = +(\mu_L - \mu_R)\bar{I}_M$ with the power dissipated by the device, the entropy production just becomes $\dot{S}_{\rm i} = \beta P_{\rm diss} \geq 0$.

2.5.3 Example: The quantum absorbtion refrigerator

Consider a three-level system

$$H_S = 0\,|0\rangle\langle 0| + \delta\,|1\rangle\langle 1| + \Delta\,|2\rangle\langle 2|\ , \tag{2.13}$$

where the different transitions are driven by different reservoirs

$$
\begin{aligned}
S_c &= |0\rangle\langle 1| + |1\rangle\langle 0| \,, \qquad & B_c &= \sum_q h_{qc} b_{qc} + \text{h.c.} \,, \\
S_h &= |0\rangle\langle 2| + |2\rangle\langle 0| \,, \qquad & B_h &= \sum_q h_{qh} b_{qh} + \text{h.c.} \,, \\
S_w &= |1\rangle\langle 2| + |2\rangle\langle 1| \,, \qquad & B_w &= \sum_q h_{qw} b_{qw} + \text{h.c.} \,,
\end{aligned}
\tag{2.14}
$$

where the bosonic operators $b_{q\nu}$ annihilate a boson of mode q in reservoir ν. The corresponding rate matrix becomes

$$
\mathcal{L}_{\text{pop}} = \begin{pmatrix} -[\ldots] & \Gamma_c(1+n_c) & \Gamma_h(1+n_h) \\ \Gamma_c n_c & -[\ldots] & \Gamma_w(1+n_w) \\ \Gamma_h n_h & \Gamma_w n_w & -[\ldots] \end{pmatrix} \,,
\tag{2.15}
$$

which again decomposes additively in the reservoirs. Without ever explicitly calculating a current, one can see that to cool the coldest reservoir (we assume $\beta_c > \beta_h > \beta_w$), we have to traverse the cycle on average as $\rho_{00} \to \rho_{11} \to \rho_{22} \to \rho_{00}$. This implies bounds on the transition rates and stationary populations

$$
\begin{aligned}
\Gamma_c n_c \bar\rho_{00} &> \Gamma_c(1+n_c)\bar\rho_{11} \,, \\
\Gamma_w n_w \bar\rho_{11} &> \Gamma_w(1+n_w)\bar\rho_{22} \,, \\
\Gamma_h(1+n_h)\bar\rho_{22} &> \Gamma_h n_h \bar\rho_{00} \,.
\end{aligned}
\tag{2.16}
$$

Multiplying the inequalities yields $n_c n_w(1+n_h) > (1+n_c)(1+n_w)n_h$, which can be rewritten as

$$
\frac{n_c}{1+n_c}\frac{n_w}{1+n_w} > \frac{n_h}{1+n_h} \,,
\tag{2.17}
$$

which upon taking the natural logarithm becomes

$$
+\beta_c\delta + \beta_w(\Delta - \delta) < +\beta_h\Delta \,,
\tag{2.18}
$$

which defines an operational window of cooling

$$
\beta_c \in \left(\beta_h, \beta_h\frac{\Delta}{\delta} - \beta_w\frac{\Delta-\delta}{\delta}\right) \,,
\tag{2.19}
$$

which is non-vanishing whenever $\beta_h > \beta_w$.