物性理論IV 講義ノート 5月13日 2024

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4 Master equation II

This is the lecture note on May 13, 2024 focusing on the dynamics of a single level quantum dot coupled to two particle reservoirs in local equilibria.

4.1 Extension to the particle reservoir

In the previous lecture, we considered a system with several internal states with different energies, which are made transitions by the influence of the environment. Namely, the environment can feed (extract) *energy* to (from) the system. Today, we consider the situation that the environment is also a particle reservoir, that can feed (extract) particles to (from) the system.

First, we consider a focused system with a single level of energy ϵ_0 (>0) coupled to a single reservoir. We disregard other internal degrees of freedom like spin degeneracy. The system can exchange particles with a reservoir which is in the thermal equilibrium at temperature T and the chemical potential μ. In the following, we consider two distinct states of the system, namely, the empty state with particle number $N=0$ and its energy $E^{(0)}=0$ and the filled state with particle number $N=1$ and its energy $E^{(1)}=\epsilon_0$ The transition rate γ_+ represents the process from empty to filled, and the transition rate γ_- represents the process from filled to empty. In other words, γ_+ is the process of one particle fed from the reservoir and γ_- is the process of one particle escaping to the reservoir.

The detailed balance condition is now stated as

$$\frac{\gamma_+}{\gamma_-} = e^{-\beta(\epsilon_0-\mu)}, \tag{1}$$

where $\beta = 1/(k_{\rm B}T)$. This can be understood since the transition rates are related to that of the Gibbs distribution, $\frac{1}{\Xi}e^{-\beta(E^{(N)}-\mu N)}$, and the steady state after a long time is the grand-canonical distribution of temperature T and chemical potential μ.

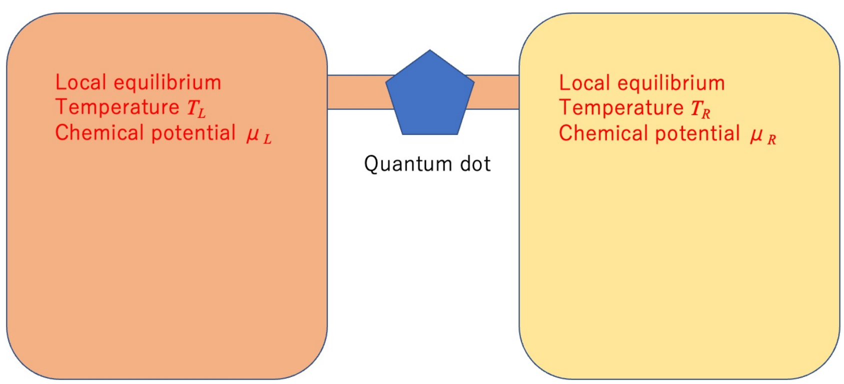

Figure 1: Model of a quantum dot coupled with two reservoirs in local equilibrium.

4.2 A system coupled to two reservoirs

We consider two reservoirs L and R, which are in local thermal equilibria with temperature $T_{L/R}$ and chemical potential $\mu_{L/R}$ as shown in Fig. 1 Accordingly, we define two transition rates, $\gamma_{L\pm}$ and $\gamma_{R\pm}$. We will study the probability distribution of the empty, $W_0(t)$, and filled $W_1(t)$ states, respectively. The conservation of the probability requires

$$W_0(t) + W_1(t) = 1, \text{ for } \forall t. \tag{2}$$

The master equation reads

$$\frac{dW_1(t)}{dt} = -\gamma_- W_1(t) + \gamma_+ W_0(t), \tag{3}$$

where we have defined total tunneling-in rate $\gamma_+ \equiv \gamma_{L+} + \gamma_{R+}$ and total tunneling-out rate $\gamma_- \equiv \gamma_{L-} + \gamma_{R-}$.

Let us move to Dirac notation, where

$$|W(t)\rangle = \begin{pmatrix} W_0(t) \\ W_1(t) \end{pmatrix}, \tag{4}$$

and the master equation becomes

$$\frac{d}{dt}|W(t)\rangle = \hat{M}|W(t)\rangle. \tag{5}$$

The transition matrix is

$$\hat{M} = \begin{pmatrix} -\gamma_+ & \gamma_- \\ \gamma_+ & -\gamma_- \end{pmatrix}. \tag{6}$$

The eigenvalues of this matrix is 0 and $-(\gamma_+ + \gamma_-)$. The eigenfunction corresponding to the steady state, $|0\rangle$ is determined by $\hat{M}|0\rangle = 0$ and normalization condition $\langle 0|0\rangle = 1$ with $\langle 0| = (1, 1)$, which is

$$|0\rangle = \frac{1}{\gamma}\begin{pmatrix} \gamma_- \\ \gamma_+ \end{pmatrix}, \tag{7}$$

where $\gamma \equiv \gamma_+ + \gamma_-$.

4.2.1 Global equilibrium

Let us study the obtained result of the steady state more in detail. Here we first consider the situation that $T_L = T_R = T$ and $\mu_L = \mu_R = \mu$, which means that the total system is in global equilibrium, hence the detail balance condition suggests

$$\frac{\gamma_+}{\gamma_-} = e^{-\beta(\epsilon_0 - \mu)}. \tag{8}$$

Hence,

$$\gamma = \gamma_+ + \gamma_- = \left\{ e^{-\beta(\epsilon_0 - \mu)} + 1 \right\} \gamma_-, \tag{9}$$

and we have

$$\gamma_- = \frac{\gamma}{1 + e^{-\beta(\epsilon_0 - \mu)}} = \gamma(1 - f(\epsilon_0)), \tag{10}$$

where we have introduced the **Fermi distribution function**

$$f(\epsilon_0) = \frac{1}{e^{\beta(\epsilon_0 - \mu)} + 1}. \tag{11}$$

And

$$\gamma_+ = e^{-\beta(\epsilon_0 - \mu)}\gamma_- = \gamma f(\epsilon_0). \tag{12}$$

Hence, the steady state reduces

$$|0\rangle = |W_{\rm st}\rangle = \frac{1}{\gamma}\left(\begin{array}{c} \gamma(1-f(\epsilon_0)) \\ \gamma f(\epsilon_0) \end{array}\right) = \left(\begin{array}{c} 1-f(\epsilon_0) \\ f(\epsilon_0) \end{array}\right). \tag{13}$$

The expectation value of the particle number in the system is

$$\langle \hat{N} \rangle = \sum_{N=0}^{1} N W_{N,\rm st} = W_{1,\rm st} = f(\epsilon_0), \tag{14}$$

which is expected from the global equilibrium condition. By the way, here it appears "Fermi distribution function". Why is the Fermi statistics ? This is related to our initial assumption that the system has only two distinct states, "empty" and "filled with one particle", but no more than one particles. This is equivalent to Pauli exclusion principle, which is the property of Fermions.

4.2.2 Bose particles

Then let us discuss what will happen when the particles obey Boson statistics. Now the probability distribution functions of distinct states of the system are $W_0(t), W_1(t), W_2(t), \ldots$ and are represented in a ket vector,

$$|W(t)\rangle = \left(\begin{array}{c} W_0(t) \\ W_1(t) \\ W_2(t) \\ \vdots \end{array}\right). \tag{15}$$

Master equation is $\frac{d}{dt}|W\rangle = \hat{M}|W\rangle$ with the transition matrix

$$\hat{M} = \left(\begin{array}{cccc} -\gamma_+ & \gamma_- & 0 & \cdots \\ \gamma_+ & -\gamma_- - \gamma_+ & \gamma_- & \cdots \\ 0 & \gamma_+ & -\gamma_- - \gamma_+ & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{array}\right). \tag{16}$$

The steady state eigenvector corresponding the eigenvalue 0 is solved by an ansatz,

$$|0\rangle = C\left(\begin{array}{c} 1 \\ e^{-\lambda} \\ e^{-2\lambda} \\ \vdots \end{array}\right), \tag{17}$$

with non-negative parameter λ and a normalization constant C. From the condition, $\hat{M}|0\rangle = 0$, we have the relation for $n=0$,

$$-C\gamma_+ + Ce^{-\lambda}\gamma_- = 0, \tag{18}$$

and $n \geq 1$,

$$Ce^{-(n-1)\lambda}\gamma_+ - Ce^{-n\lambda}(\gamma_- + \gamma_+) + Ce^{-(n+1)\lambda}\gamma_- = 0. \tag{19}$$

By introducing $x \equiv e^{\lambda}$, this is equivalent to

$$\gamma_+ x^2 - (\gamma_+ + \gamma_-)x + \gamma_- = 0, \tag{20}$$

which has a solution

$$x = \frac{\gamma_+ + \gamma_- \pm |\gamma_+ - \gamma_-|}{2\gamma_+} = 1 \ \text{ or } \ \frac{\gamma_-}{\gamma_+} \tag{21}$$

The first result ($x = 0$) is not compatible with Eq. (18). For the second result, from the detailed balance condition,

$$x = e^{\lambda} = \frac{\gamma_-}{\gamma_+} = e^{\beta(\epsilon_0 - \mu)}. \tag{22}$$

It is clear that if λ is negative ($x < 1$), the norm $1 = \langle 0|0\rangle = C \sum_{n=0}^{\infty} e^{-n\lambda}$ diverges and the results cannot be physically acceptable. This situation is corresponding to $\gamma_- < \gamma_+$ with $\epsilon_0 < \mu$, when the energy level of the quantum dot is below the chemical potential of the reservoir(s) and to establish thermal equilibrium, particles keep flowing into the quantum dot forever and the steady state is never achieved. Next, we study the case $\gamma_+ < \gamma_-$ with $\epsilon_0 > \mu$, where the steady state is normalizable $1 = \langle 0|0\rangle = C \sum_{n=0}^{\infty} e^{-n\lambda} = \frac{C}{1-e^{-\lambda}}$ and hence $C = 1 - e^{-\lambda}$. Now, we evaluate the expectation value of the total number of particles in the system,

$$\begin{aligned}
\langle \hat{N} \rangle &= \sum_{n=0}^{\infty} n W_{n,\mathrm{st}} \\
&= \left(1 - e^{-\lambda}\right) \left\{ e^{-\lambda} + 2e^{-2\lambda} + 3e^{-3\lambda} + \cdots \right\} \\
&= \frac{e^{-\lambda}}{1 - e^{-\lambda}} = \frac{1}{e^{\lambda} - 1}.
\end{aligned} \tag{23}$$

Hence the expectation value of the particles becomes **Boson distribution function** as it should be,

$$\langle \hat{N} \rangle = \frac{1}{e^{\beta(\epsilon_0 - \mu)} - 1}. \tag{24}$$

4.2.3 Local equilibria and global non-equilibrium

Let us go back to the Fermion system. We assume general non-equilibrium situations, $\mu_L \neq \mu_R$ and $T_L \neq T_R$. We assume local detailed balance conditions are satisfied:

$$\frac{\gamma_{L+}}{\gamma_{L-}} = e^{-\beta_L(\epsilon_0 - \mu_L)}, \tag{25}$$

$$\frac{\gamma_{R+}}{\gamma_{R-}} = e^{-\beta_R(\epsilon_0 - \mu_R)}, \tag{26}$$

where $\beta_{L/R} = 1/(k_{\mathrm{B}} T_{L/R})$. With defining $\gamma_L = \gamma_{L+} + \gamma_{L-}$ and $\gamma_R = \gamma_{R+} + \gamma_{R-}$, we can fix four rates $\gamma_{L/R,\pm}$ using Fermi distribution functions ($\nu = L/R$)

$$f_\nu(\epsilon_0) = \frac{1}{e^{\beta_\nu(\epsilon_0 - \mu_\nu)} + 1}. \tag{27}$$

The total tunneling-in and tunneling-out rates are

$$\gamma_+ = \gamma_L f_L(\epsilon_0) + \gamma_R f_R(\epsilon_0), \tag{28}$$

$$\gamma_- = \gamma_L(1 - f_L(\epsilon_0)) + \gamma_R(1 - f_R(\epsilon_0)), \tag{29}$$

respectively. Then the steady state (not in equilibrium, but non-equilibrium steady state; NESS) is

$$|W_{\mathrm{st}}\rangle = |0\rangle = \frac{1}{\gamma} \begin{pmatrix} \gamma_- \\ \gamma_+ \end{pmatrix}, \tag{30}$$

where $\gamma \equiv \gamma_+ + \gamma_- = \gamma_L + \gamma_R$. In particular, the probability that the system is filled in the steady state is

$$W_{\mathrm{st},1} = \frac{\gamma_L f_L(\epsilon_0) + \gamma_R f_R(\epsilon_0)}{\gamma_L + \gamma_R}. \tag{31}$$

In Fig. 2, we plot $W_{\mathrm{st},1} \equiv \langle \hat{N} \rangle$ as a function of ϵ_0 for a set of fixed parameters.

Exercise III: Plot the probability $W_{\mathrm{st},1}$ as a function of ϵ_0/γ when $\gamma_L = \gamma_R \equiv \gamma$, $\mu_L = \mu_R = 0$, and $\beta_L = 0.2/\gamma$ and $\beta_R = 5/\gamma$. Then provide physical explanation of the obtained result.

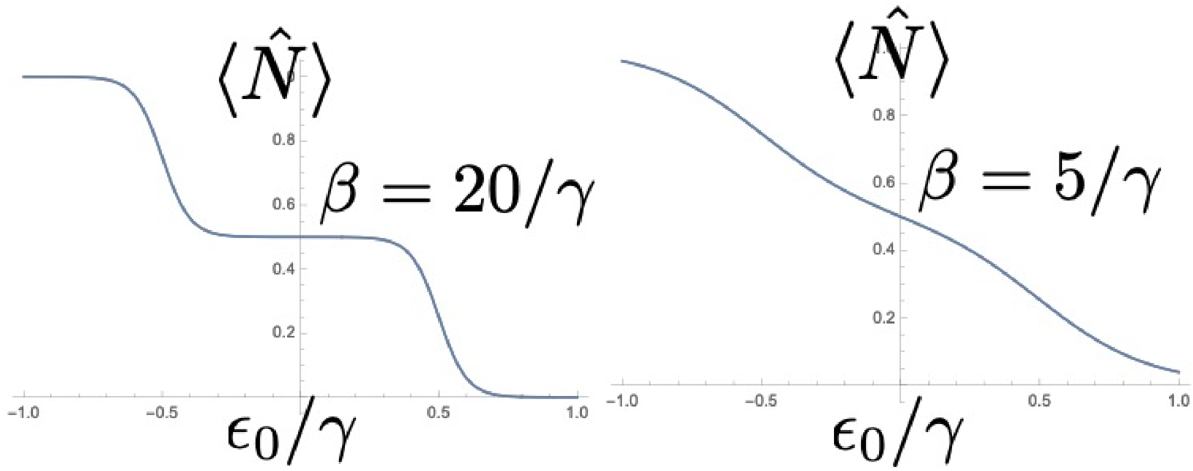

Figure 2: The probability that the system is filled as a function of the level energy for $\gamma_L = \gamma_R \equiv \gamma$, $\mu_L = \gamma/2$, $\mu_R = -\gamma/2$ and $\hbar = 1$. Left: Low temperature behavior: $\beta = 20/\gamma$, Right: High temperature behavior: $\beta = 5/\gamma$.

4.2.4 Current

Since the total system is not in equilibrium, there can be some flow of particles. From the system to the right reservoir, the particle **flux (current)** is defined by

$$I_R(t) = W_1(t)\gamma_{R-} - W_0(t)\gamma_{R+}, \tag{32}$$

and the flux from the system to the left reservoir is

$$I_L(t) = W_1(t)\gamma_{L-} - W_0(t)\gamma_{L+}. \tag{33}$$

The total flux from the system to the environment is

$$I_R(t) + I_L(t) = W_1(t)\gamma_{-} - W_0(t)\gamma_{+}. \tag{34}$$

This is related to the change of the occupation of the system

$$\begin{aligned} \frac{d}{dt}\langle \hat{N} \rangle = \frac{d}{dt}W_1(t) &= -\gamma_- W_1(t) + \gamma_+ W_0(t) \\ &= -I_R(t) - I_L(t). \end{aligned} \tag{35}$$

This is understood as the continuity relation,

$$\frac{d}{dt}\rho(t) + \mathrm{div}\vec{j}(t) = 0, \tag{36}$$

where particle density is $\rho(t) = \langle \hat{N} \rangle / (\Delta x)^3$ and the current density $j_\nu(t) = I_\nu(t)/(\Delta x)^2$ where Δx is some certain length characterizing the size of the system. We used the relation $\mathrm{div}\vec{j}(t) = \frac{dj_x(t)}{dx} = \frac{j_R(t) - \{-j_L(t)\}}{\Delta x} = \frac{1}{(\Delta x)^3}\{I_R(t) + I_L(t)\}$.

In the steady state condition,

$$\frac{d\langle \hat{N} \rangle}{dt} = \frac{dW_{\mathrm{st},1}}{dt} = 0, \tag{37}$$

and

$$
\begin{aligned}
I_{\mathrm{st}R} &= -I_{\mathrm{st}L} = W_{\mathrm{st},1}\gamma_{R-} - W_{\mathrm{st},0}\gamma_{R+} \\
&= \frac{\gamma_+}{\gamma}\gamma_R(1 - f_R(\epsilon_0)) - \frac{\gamma_-}{\gamma}\gamma_R f_R(\epsilon_0) \\
&= \frac{1}{\gamma}\left[\{\gamma_L f_L(\epsilon_0) + \gamma_R f_R(\epsilon_0)\}\gamma_R(1 - f_R(\epsilon_0)) - \{\gamma_L(1 - f_L(\epsilon_0)) + \gamma_R(1 - f_R(\epsilon_0))\}\gamma_R f_R(\epsilon_0)\right] \\
&= \frac{\gamma_L\gamma_R}{\gamma}\{f_L(\epsilon_0)(1 - f_R(\epsilon_0)) - (1 - f_L(\epsilon_0))f_R(\epsilon_0)\} \\
&= \frac{\gamma_L\gamma_R}{\gamma_L + \gamma_R}\{f_L(\epsilon_0) - f_R(\epsilon_0)\}\,. \qquad (38)
\end{aligned}
$$

The ϵ_0 dependence of the current in the steady state is depicted in Fig. 3. As is evident from the results, finite steady current flows when the energy level locates in the energy window $\mu_R < \epsilon_0 < \mu_L$ at lower temperatures.

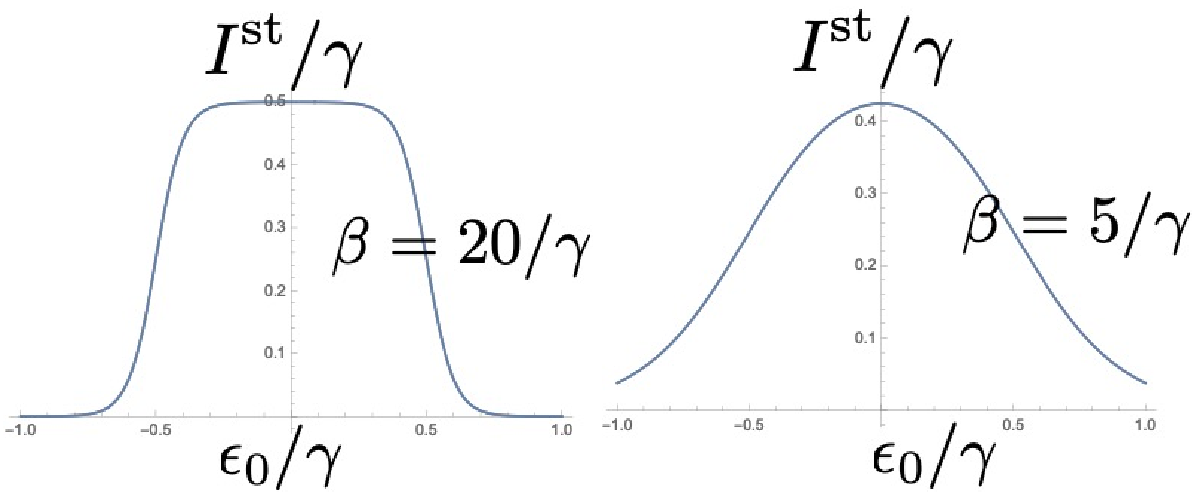

Figure 3: Steady current as a function of the level energy for $\gamma_L = \gamma_R \equiv \gamma$, $\mu_L = \gamma/2$, $\mu_R = -\gamma/2$ and $\hbar = 1$. Left: Low temperature behavior: $\beta = 20/\gamma$, Right: High temperature behavior: $\beta = 5/\gamma$.

Exercise IV: Plot steady state current I^{st}/γ as a function of ϵ_0/γ when $\gamma_L = \gamma_R \equiv \gamma$, $\mu_L = \mu_R = 0$, and $\beta_L = 0.2/\gamma$ and $\beta_R = 5/\gamma$. Then provide physical explanation of the obtained result.

4.3 Conclusion

We have extended the master equation for the system with exchanging particles with fermionic or bosonic reservoirs. When the system is coupled to two reservoirs with global non-equilibrium situation, system can achieve a steady state accompanying a steady flow of particles. It is important to understand that the current discussed today is the average current. In fact, from a microscopic viewpoint, the current is made of the flow of many particles and is in fact fluctuating in time. In the next lecture, we will consider the fluctuation of the current, or equivalently, the *current noise*.