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8 Quantum master equation

This is a lecture note of the theory of condensed matter IV, on Jun. 10 concerning the derivation of the quantum master equation of a single level quantum dot for a spinless electron system coupled to two reservoirs. We show that the quantum master equation can be reduced to the GKSL (Lindblad) form, whose diagonal components are equivalent to the classical master equation that we had discussed.

8.1 Model

We define the Hamiltonian, $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_1$, where the unperturbed part is made of Hamiltonians of a quantum dot (QD) and of reservoirs, *i.e.*, $\hat{\mathcal{H}}_0 = \hat{\mathcal{H}}_{\rm dot} + \hat{\mathcal{H}}_{\rm res}$. We consider the simplest model Hamiltonian of the QD system, $\hat{\mathcal{H}}_{\rm dot} = \epsilon_0 \hat{n}$, where the electron number operator in the QD is defined by $\hat{n} = \hat{d}^\dagger \hat{d}$ using QD spinless creation (annihilation) operator $\hat{d}^\dagger(\hat{d})$ satisfying Fermionic anticommutation relation $\left\{\hat{d}, \hat{d}^\dagger\right\} = 1$. Here we assume two reservoirs, left (L) and right (R), as shown in Fig. 1, $\hat{\mathcal{H}}_{\rm res} = \sum_\alpha \hat{\mathcal{H}}_\alpha$. The Hamiltonian of the reservoir $\alpha = L/R$ is

$$\hat{\mathcal{H}}_\alpha = \sum_k \varepsilon_k \hat{C}^\dagger_{\alpha k} \hat{C}_{\alpha k}, \tag{1}$$

where k is the quasi-continuous quantum number in each reservoir and $\hat{C}^\dagger_{\alpha k}(\hat{C}_{\alpha k})$ is the creation (annihilation) operator of the reservoir α, satisfying the anti-commutation relation $\left\{\hat{C}_{\alpha k}, \hat{C}^\dagger_{\alpha' k'}\right\} = \delta_{\alpha\alpha'}\delta_{kk'}$.

The perturbation term is the tunnel couplings

$$\hat{\mathcal{H}}_1 = \sum_{\alpha k} (V_{\alpha k} \hat{C}^\dagger_{\alpha k} \hat{d} + \text{H.c.}), \tag{2}$$

where the complex coupling constants $V_{\alpha k}$ are introduced and "H.c." depicts the Hermite conjugate.

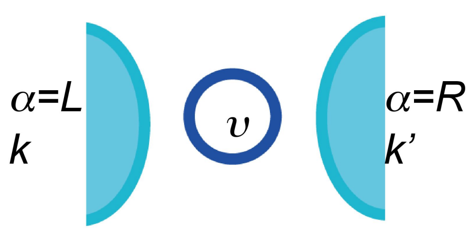

Figure 1: Model of the system considered in this note.

8.2 Interaction picture and Green functions

In the following, we use a unit system $\hbar = 1$. Let us introduce an interaction picture of a generic operator $\hat{\mathcal{O}}$, signified by a symbol 'tilde', $\tilde{\mathcal{O}}(t) \equiv e^{i\hat{\mathcal{H}}_0 t}\hat{\mathcal{O}} e^{-i\hat{\mathcal{H}}_0 t}$. Since we assume non-interacting reservoirs, the interaction picture of the annihilation/creation operators are[1]

$$\tilde{C}_{\alpha k}(t) = e^{-i\varepsilon_k t}\hat{C}_{\alpha k}, \quad \tilde{C}^\dagger_{\alpha k}(t) = e^{i\varepsilon_k t}\hat{C}^\dagger_{\alpha k}. \tag{4}$$

Green functions are versatile tool in physics. For example, the general solution to the Poisson equation can be obtained by a Green function, $G(\boldsymbol{r}, \boldsymbol{r}') = -1/|\boldsymbol{r} - \boldsymbol{r}'|$. They are also quite useful in analyzing dynamics of quantum many-body system. Here we introduce retarded/advanced and lesser/greater Green functions. These four Green functions are also very important in the discussions of non-equilibrium physics, since Keldysh or non-equilibrium Green function, that will be discussed in the next lecture, is made of these Green functions. In the linear response formalism, time-ordered Green function is also important.

First we define the **retarded Green function** of the reservoir α as

$$\mathcal{G}^R_\alpha(k,t) \equiv -i\theta(t)\left\langle\{\tilde{C}_{\alpha k}(t), \tilde{C}^\dagger_{\alpha k}(0)\}\right\rangle_0, \tag{5}$$

where $\theta(t)$ is the Heaviside step function and $\left\{\hat{A}, \hat{B}\right\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ is the anticommutator. The thermal average (for reserviors in local equilibria) is defined by

$$\langle\hat{\mathcal{O}}\rangle_0 \equiv \mathrm{Tr}\left\{\hat{\chi}_0\hat{\mathcal{O}}\right\}, \tag{6}$$

with the symbol Tr representing the trace and

$$\hat{\chi}_0 = \hat{\chi}(t_0) = \prod_\alpha \frac{e^{-\beta(\hat{\mathcal{H}}_\alpha - \mu_\alpha\hat{\mathcal{N}}_\alpha)}}{\mathrm{Tr}\left\{e^{-\beta(\hat{\mathcal{H}}_\alpha - \mu_\alpha\hat{\mathcal{N}}_\alpha)}\right\}} \otimes \hat{\rho}_0 = \hat{R}_0 \otimes \hat{\rho}_0, \tag{7}$$

is the initial (at time $t = t_0$) density matrix of all system. Here, $\hat{R}_0$ is the density operator of the reservoirs where $\beta = 1/(k_\mathrm{B}T)$ with the Boltzmann's constant k_B and the bath temperature T assumed to be common in all reservoirs. (This condition can be easily generalized for any local equilibria with different temperatures.) μ_α is the chemical potential and $\hat{\mathcal{N}}_\alpha \equiv \sum_k \hat{C}^\dagger_{\alpha k}\hat{C}_{\alpha k}$ is the total electron number operator of the reservoir α. $\hat{\rho}_0$ is an arbitrary initial density operator of the QD system. Since the average is over thermal equilibrium reservoirs, $\mathcal{G}^R_\alpha(k,t)$ is only the function of time difference of two operators, $\tilde{C}_{\alpha k}(t)$ and $\tilde{C}^\dagger_{\alpha k}(0)$. Using Eq. (4), we obtain an explicit form

$$\mathcal{G}^R_{\alpha k}(k,t) = -i\theta(t)e^{-i\varepsilon_k t}, \tag{8}$$

and its Fourier transform is

$$\mathcal{G}^R_\alpha(k,\omega) \equiv \int_{-\infty}^{\infty} dt e^{i\omega t}\mathcal{G}^R_\alpha(k,t) = \frac{1}{\omega - \varepsilon_k + i\eta} = \mathcal{P}\frac{1}{\omega - \varepsilon_k} - i\pi\delta(\omega - \varepsilon_k), \tag{9}$$

where a positive infinitesimal η is introduced to make the integral converge and the last expression includes Cauchy's principle integral and the Dirac's delta function. The **advanced Green function** is defined by

$$\mathcal{G}^A_\alpha(k,t) \equiv i\theta(-t)\left\langle\{\tilde{C}_{\alpha k}(t), \tilde{C}^\dagger_{\alpha k}(0)\}\right\rangle_0, \tag{10}$$

and whose Fourier transform $\mathcal{G}^A_\alpha(k,\omega)$ is a complex conjugate of $\mathcal{G}^R_\alpha(k,\omega)$.

We also define the **lesser Green function** of the reservoir α

$$\mathcal{G}^<_\alpha(k,t) \equiv i\left\langle\tilde{C}^\dagger_{\alpha k}\tilde{C}_{\alpha k}(t)\right\rangle_0 = ie^{-i\varepsilon_k t}\left\langle\hat{C}^\dagger_{\alpha k}\hat{C}_{\alpha k}\right\rangle_0 = ie^{-i\varepsilon_k t}f_\alpha(\varepsilon_k), \tag{11}$$

where we introduced the Fermi distribution function of the reservoir α:

$$f_\alpha(\varepsilon) = \frac{1}{e^{\beta(\varepsilon - \mu_\alpha)} + 1}. \tag{12}$$

[1] The derivation is as follows: the Heisenberg equation of motion of $\tilde{C}_{\alpha k}(t)$ is

$$\frac{d\tilde{C}_{\alpha k}(t)}{dt} = e^{i\hat{\mathcal{H}}_0 t} i\left[\hat{\mathcal{H}}_0, \hat{C}_{\alpha k}\right] e^{-i\hat{\mathcal{H}}_0 t} = -i\varepsilon_k\tilde{C}_{\alpha k}(t), \tag{3}$$

with the initial condition $\tilde{C}_{\alpha k}(t = 0) = \hat{C}_{\alpha k}$. Hence, the solution is $\tilde{C}_{\alpha k}(t) = e^{-i\varepsilon_k t}\hat{C}_{\alpha k}$. The result of $\tilde{C}^\dagger_{\alpha k}(t)$ is obtained by taking the Hermite conjugate of $\tilde{C}_{\alpha k}(t)$.

Again, lesser Green function of the reservoir α is also a function of the time difference of the operators.[2] The Fourier transform of the lesser Green function is

$$\mathcal{G}^{<}_{\alpha}(k,\omega) = iA_{\alpha}(k,\omega) f_{\alpha}(\varepsilon_k), \tag{13}$$

where $A_{\alpha}(k,\omega)$ is the **spectral function** of the reservoir α and is proportional to the Dirac's delta-function for free (non-interacting) reservoir $A_{\alpha}(k,\omega) \equiv 2\pi\delta(\omega - \varepsilon_k)$. Similarly, we introduce the **greater Green function**

$$\mathcal{G}^{>}_{\alpha}(k,t) = -i \langle \tilde{C}_{\alpha k}(t) \tilde{C}^{\dagger}_{\alpha k} \rangle_0 \tag{14}$$

and its Fourier transform is

$$\mathcal{G}^{>}_{\alpha}(k,\omega) = -iA_{\alpha}(k,\omega) \tilde{f}_{\alpha}(\varepsilon_k), \tag{15}$$

where we defined hole distribution function $\tilde{f}_{\alpha}(\varepsilon) \equiv 1 - f_{\alpha}(\varepsilon)$.

8.3 Density matrix

The total system density matrix at time t is

$$\hat{\chi}(t) = e^{-i\hat{\mathcal{H}}t} \hat{\chi}(t_0) e^{i\hat{\mathcal{H}}t}, \tag{16}$$

and its equation of motion (Liouville von Neumann equation) is

$$\frac{d}{dt}\hat{\chi}(t) = -i[\hat{\mathcal{H}}, \hat{\chi}(t)]. \tag{17}$$

Moving to the interaction picture $\tilde{\chi}(t)$ and the equation of motion becomes

$$\frac{d}{dt}\tilde{\chi}(t) = -i[\tilde{\mathcal{H}}_1(t), \tilde{\chi}(t)], \tag{18}$$

where the interaction Hamiltonian in the interaction picture is

$$\tilde{\mathcal{H}}_1(t) \equiv e^{i\hat{\mathcal{H}}_0 t} \hat{\mathcal{H}}_1 e^{-i\hat{\mathcal{H}}_0 t}. \tag{19}$$

Equation (18) has a general formal solution:

$$\tilde{\chi}(t) = \tilde{\chi}(t_0) - i\int_{t_0}^{t} dt' [\tilde{\mathcal{H}}_1(t'), \tilde{\chi}(t')], \tag{20}$$

where $\tilde{\chi}(t_0) = \hat{\chi}_0$ is the initial density matrix of total system. With putting Eq. (20) into Eq. (18), we obtain

$$\frac{d}{dt}\tilde{\chi}(t) = -i[\tilde{\mathcal{H}}_1(t), \hat{\chi}_0] - \int_{t_0}^{t} dt' [\tilde{\mathcal{H}}_1(t), [\tilde{\mathcal{H}}_1(t'), \tilde{\chi}(t')]]. \tag{21}$$

The density matrix of the system (QD) is defined by

$$\tilde{\rho}(t) \equiv \mathrm{Tr}_{\mathrm{res}} \tilde{\chi}(t), \tag{22}$$

where $\mathrm{Tr}_{\mathrm{res}}$ represents the partial trace on the reservoir degree of freedom. Principle approximation resides in replacing $\tilde{\chi}(t')$ in the integral kernel by $\hat{R}_0 \otimes \tilde{\rho}(t)$ (Born-Markov approximation). Since the tunneling Hamiltonian $\hat{\mathcal{H}}_1$ contains single annihilation or creation operator of the reservoir, it is obvious that $\mathrm{Tr}_{\mathrm{res}}[\tilde{\mathcal{H}}_1(t), \hat{\chi}_0] = 0$. Now taking the partial trace of Eq. (21) provides the final expression (Redfield equation):

$$\frac{d}{dt}\tilde{\rho}(t) = -\int_{t_0}^{t} dt' \mathrm{Tr}_{\mathrm{res}} [\tilde{\mathcal{H}}_1(t), [\tilde{\mathcal{H}}_1(t'), \hat{R}_0 \otimes \tilde{\rho}(t)]], \tag{23}$$

which represents *sequential tunnel process*.

[2] In fact, the retarded and lesser Green functions of the QD, defined as

$$\mathcal{G}^{R}_{\mathrm{dot}}(t,t') \equiv -i\theta(t-t') \langle \left\{ \tilde{d}(t), \tilde{d}^{\dagger}(t') \right\} \rangle_0 ,$$

$$\mathcal{G}^{<}_{\mathrm{dot}}(t,t') \equiv i \langle \tilde{d}^{\dagger}(t') \tilde{d}(t) \rangle_0 ,$$

which do not appear in the discussion of today, are not in general the function of the time difference, $t - t'$, but explicitly depends on both times t and t'. This is because the initial quantum state of the electrons in QD $\hat{\rho}_0$ is not necessarily commutes with $\hat{\mathcal{H}}_{\mathrm{dot}}$.

8.4 Quantum master equation

This section explicitly evaluates the Redfield equation derived in the previous section. We change the variable in Eq. (23) from t' to $\tau \equiv t - t'$ and $\int_{t_0}^{t} dt' \to \int_0^{t-t_0} d\tau$. It can be shown that the integral kernel of Eq. (23) is a rapidly decaying function of τ. Using the characteristic relaxation time of the reservoir, $\tau_{\rm rel}$, for $t - t_0 \gg \tau_{\rm rel}$ we can safely extend the upper limit of the integral to ∞ if we are interested in a steady state property (not the transient property). Then,

$$\begin{aligned}
\frac{d\tilde{\rho}(t)}{dt} &= -\int_0^\infty d\tau \mathrm{Tr}_{\rm res}[\tilde{\mathcal{H}}_1(t), [\tilde{\mathcal{H}}_1(t-\tau), \hat{R}_0 \otimes \tilde{\rho}(t)]] \\
&= -\int_0^\infty d\tau \mathrm{Tr}_{\rm res}\{\tilde{\mathcal{H}}_1(t)\tilde{\mathcal{H}}_1(t-\tau)\hat{R}_0 \otimes \tilde{\rho}(t) && (24)\\
&\qquad - \tilde{\mathcal{H}}_1(t)\hat{R}_0 \otimes \tilde{\rho}(t)\tilde{\mathcal{H}}_1(t-\tau) && (25)\\
&\qquad - \tilde{\mathcal{H}}_1(t-\tau)\hat{R}_0 \otimes \tilde{\rho}(t)\tilde{\mathcal{H}}_1(t) && (26)\\
&\qquad + \hat{R}_0 \otimes \tilde{\rho}(t)\tilde{\mathcal{H}}_1(t-\tau)\tilde{\mathcal{H}}_1(t)\}. && (27)
\end{aligned}$$

Let us first evaluate Eq. (24) noting that $\mathrm{Tr}_{\rm res}\left\{\hat{C}^\dagger_{\alpha k}\hat{C}^\dagger_{\beta k'}\hat{R}_0\right\} = \mathrm{Tr}_{\rm res}\left\{\hat{C}_{\alpha k}\hat{C}_{\beta k'}\hat{R}_0\right\} = 0$,

$$\begin{aligned}
\text{(i)} &= -\int_0^\infty d\tau \mathrm{Tr}_{\rm res}\Big[\sum_{\alpha k}\left\{V_{\alpha k}\tilde{C}^\dagger_{\alpha k}(t)\hat{d}(t) + V^*_{\alpha k}\tilde{C}_{\alpha k}(t)\hat{d}^\dagger(t)\right\}\sum_{\beta k'}\left\{V_{\beta k'}\tilde{C}^\dagger_{\beta k'}(t-\tau)\hat{d}(t-\tau) + V^*_{\beta k'}\tilde{C}_{\beta k'}(t-\tau)\hat{d}^\dagger(t-\tau)\right\} \\
&\qquad \times \hat{R}_0 \otimes \tilde{\rho}(t)\Big] \\
&= -\sum_{\alpha\beta k k'}\int_0^\infty d\tau \mathrm{Tr}_{\rm res}\Big[\Big\{V_{\alpha k}V^*_{\beta k'}\tilde{C}^\dagger_{\alpha k}(t)\tilde{C}_{\beta k'}(t-\tau)\hat{d}(t)\hat{d}^\dagger(t-\tau) + V^*_{\alpha k}V_{\beta k'}\tilde{C}_{\alpha k}(t)\tilde{C}^\dagger_{\beta k'}(t-\tau)\hat{d}^\dagger(t)\hat{d}(t-\tau)\Big\} \\
&\qquad \times \hat{R}_0 \otimes \tilde{\rho}(t)\Big] \\
&= i\sum_{\alpha k}\int_0^\infty d\tau \int \frac{d\omega}{2\pi}\{V_{\alpha k}V^*_{\alpha k}e^{i\omega\tau}\mathcal{G}^<_\alpha(k,\omega)\tilde{d}(t)\tilde{d}^\dagger(t-\tau)\tilde{\rho}(t) - V^*_{\alpha k}V_{\alpha k}e^{-i\omega\tau}\mathcal{G}^>_\alpha(k,\omega)\tilde{d}^\dagger(t)\tilde{d}(t-\tau)\tilde{\rho}(t)\},
\end{aligned} \tag{28}$$

where we note that at equilibrium, the statistical average is only the function of the time difference, namely, $\mathrm{Tr}_{\rm res}\left\{\tilde{C}^\dagger_{\alpha k}(t)\tilde{C}_{\beta k'}(t-\tau)\hat{R}_0\right\} = \delta_{\alpha\beta}\delta_{kk'}\left\langle\tilde{C}^\dagger_{\alpha k}\tilde{C}_{\alpha k}(-\tau)\right\rangle_0 = -i\delta_{\alpha\beta}\delta_{kk'}\mathcal{G}^<_\alpha(k,-\tau)$. We also note that the system Hamiltonian $\hat{\mathcal{H}}_{\rm dot}$ is diagonalized with many electron basis as follows:

$$\hat{\mathcal{H}}_{\rm dot}\left|\mathcal{N}\right\rangle = E_{\mathcal{N}}\left|\mathcal{N}\right\rangle, \tag{29}$$

where $\mathcal{N}$ is the total number of electrons in the QD system. We depict a quantum number m, n representing $\mathcal{N} = 0, 1$. With inserting complete sets p like $1 = \sum_p |p\rangle\langle p|$, the m, n matrix element is

$$\begin{aligned}
\langle m|\text{(i)}|n\rangle &= i\sum_{\alpha k}|V_{\alpha k}|^2\int_0^\infty d\tau\int\frac{d\omega}{2\pi}\sum_{pq} \\
&\times\Big\{e^{i\omega\tau}\mathcal{G}^<_\alpha(k,\omega)e^{iE_m t}\langle m|\hat{d}|p\rangle e^{-iE_p t}e^{iE_p(t-\tau)}\langle p|\hat{d}^\dagger|q\rangle e^{-iE_q(t-\tau)}e^{iE_q t}\hat{\rho}(t)e^{-iE_n t} \\
&- e^{-i\omega\tau}\mathcal{G}^>_\alpha(k,\omega)e^{iE_m t}\langle m|\hat{d}^\dagger|p\rangle e^{-iE_p t}e^{iE_p(t-\tau)}\langle p|\hat{d}|q\rangle e^{-iE_q(t-\tau)}e^{iE_q t}\hat{\rho}(t)e^{-iE_n t}\Big\} \\
&= i\sum_{\alpha k}|V_{\alpha k}|^2\int_0^\infty d\tau\int\frac{d\omega}{2\pi}\sum_{pq}e^{i(E_m-E_n)t} \\
&\times\Big\{2\pi i\delta(\omega-\varepsilon_k)f_\alpha(\varepsilon_k)e^{i(\omega-E_p+E_q)\tau}\langle m|\hat{d}|p\rangle\langle p|\hat{d}^\dagger|q\rangle\rho_{qn(t)} \\
&+ 2\pi i\delta(\omega-\varepsilon_k)\tilde{f}_\alpha(\varepsilon_k)e^{i(-\omega-E_p+E_q)\tau}\langle m|\hat{d}^\dagger|p\rangle\langle p|\hat{d}|q\rangle\rho_{qn(t)}\Big\}.
\end{aligned} \tag{30}$$

In the last step, we executed the τ integral like

$$\int_0^\infty d\tau e^{i(\Omega+i\eta)\tau} = \frac{i}{\Omega+i\eta} \approx \pi\delta(\Omega), \tag{31}$$

where we introduced the positive infinitesimal η to make the integral converge and we neglected the contribution of the principle integral. Usually the summation on wave numbers can be replaced with the integration in energy with introducing the **line-width function**: for an arbitrary function of reservoir energy ε_k, $F(\varepsilon_k)$,

$$\sum_{\alpha k} V_{\alpha k} V_{\alpha k}^* F(\varepsilon_k) = \sum_{\alpha k} V_{\alpha k} V_{\alpha k}^* \int d\epsilon F(\epsilon)\delta(\epsilon - \varepsilon_k) = \sum_{\alpha} \int d\epsilon F(\epsilon) \sum_{k} V_{\alpha k} V_{\alpha k}^* \delta(\epsilon - \varepsilon_k) = \sum_{\alpha} \int \frac{d\epsilon}{2\pi} \Gamma_\alpha(\epsilon) F(\epsilon), \tag{32}$$

where $\Gamma_\alpha(\epsilon) \equiv 2\pi \sum_k V_{\alpha k} V_{\alpha k}^* \delta(\epsilon - \varepsilon_k)$ is the line-width function[1] and we neglect its energy dependence (wide-band limit) in the following arguments. Then we have

$$\begin{aligned}\langle m|(\mathrm{i})|n\rangle = {}& ie^{i(E_m-E_n)t} \sum_{\alpha} \int \frac{d\epsilon}{2\pi} \Gamma_\alpha(\epsilon) \sum_{pq} \pi i \\ &\times \Big\{ \delta(\epsilon - E_p + E_q) f_\alpha(\epsilon) \langle m|\hat{d}|p\rangle \langle p|\hat{d}^\dagger|q\rangle \rho_{qn}(t) + \delta(\epsilon + E_p - E_q) \tilde{f}_\alpha(\epsilon) \langle m|\hat{d}^\dagger|p\rangle \langle p|\hat{d}|q\rangle \rho_{qn}(t) \Big\}.\end{aligned} \tag{33}$$

Similarly, Eq. (25) is

$$(\mathrm{ii}) = i \sum_{\alpha k} \int_0^\infty d\tau \int \frac{d\omega}{2\pi} \{ V_{\alpha k} V_{\alpha k}^* e^{i\omega\tau} \mathcal{G}_\alpha^>(k,\omega) \tilde{d}(t) \tilde{\rho}(t) \tilde{d}^\dagger(t-\tau) - V_{\alpha k}^* V_{\alpha k} e^{-i\omega\tau} \mathcal{G}_\alpha^<(k,\omega) \tilde{d}^\dagger(t) \tilde{\rho}(t) \tilde{d}(t-\tau) \}, \tag{34}$$

and m, n matrix element is

$$\begin{aligned}\langle m|(\mathrm{ii})|n\rangle = {}& ie^{i(E_m-E_n)t} \sum_{\alpha} \int \frac{d\epsilon}{2\pi} \Gamma_\alpha(\epsilon) \sum_{pq} (-\pi i) \\ &\times \Big\{ \delta(\epsilon - E_q + E_n) \tilde{f}_\alpha(\epsilon) \langle m|\hat{d}|p\rangle \rho_{pq}(t) \langle q|\hat{d}^\dagger|n\rangle + \delta(\epsilon + E_q - E_n) f_\alpha(\epsilon) \langle m|\hat{d}^\dagger|p\rangle \rho_{pq}(t) \langle q|\hat{d}|n\rangle \Big\}.\end{aligned} \tag{35}$$

Equation (26) is

$$(\mathrm{iii}) = i \sum_{\alpha k} \int_0^\infty d\tau \int \frac{d\omega}{2\pi} \{ V_{\alpha k} V_{\alpha k}^* e^{-i\omega\tau} \mathcal{G}_\alpha^>(k,\omega) \tilde{d}(t-\tau) \tilde{\rho}(t) \tilde{d}^\dagger(t) - V_{\alpha k}^* V_{\alpha k} e^{i\omega\tau} \mathcal{G}_\alpha^<(k,\omega) \tilde{d}^\dagger(t-\tau) \tilde{\rho}(t) \tilde{d}(t) \}. \tag{36}$$

and m, n matrix element is

$$\begin{aligned}\langle m|(\mathrm{iii})|n\rangle = {}& ie^{i(E_m-E_n)t} \sum_{\alpha} \int \frac{d\epsilon}{2\pi} \Gamma_\alpha(\epsilon) \sum_{pq} (-i\pi) \\ &\times \Big\{ \delta(\epsilon + E_m - E_p) \tilde{f}_\alpha(\epsilon) \langle m|\hat{d}|p\rangle \rho_{pq}(t) \langle q|\hat{d}^\dagger|n\rangle + \delta(\epsilon - E_m + E_p) f_\alpha(\epsilon) \langle m|\hat{d}^\dagger|p\rangle \rho_{pq}(t) \langle q|\hat{d}|n\rangle \Big\}.\end{aligned} \tag{37}$$

Finally, Eq. (27) is

$$(\mathrm{iv}) = i \sum_{\alpha k} \int_0^\infty d\tau \int \frac{d\omega}{2\pi} \{ V_{\alpha k} V_{\alpha k}^* e^{-i\omega\tau} \mathcal{G}_\alpha^<(k,\omega) \tilde{\rho}(t) \tilde{d}(t-\tau) \tilde{d}^\dagger(t) - V_{\alpha k}^* V_{\alpha k} e^{i\omega\tau} \mathcal{G}_\alpha^>(k,\omega) \tilde{\rho}(t) \tilde{d}^\dagger(t-\tau) \tilde{d}(t) \}. \tag{38}$$

and m, n matrix element is

$$\begin{aligned}\langle m|(\mathrm{iv})|n\rangle = {}& ie^{i(E_m-E_n)t} \sum_{\alpha} \int \frac{d\epsilon}{2\pi} \Gamma_\alpha(\epsilon) \sum_{pq} \pi i \\ &\times \Big\{ \delta(\epsilon + E_p - E_q) f_\alpha(\epsilon) \rho_{mp}(t) \langle p|\hat{d}|q\rangle \langle q|\hat{d}^\dagger|n\rangle\, \delta(\epsilon - E_p + E_q) \tilde{f}_\alpha(\epsilon) \rho_{mp}(t) \langle p|\hat{d}^\dagger|q\rangle \langle q|\hat{d}|n\rangle \Big\}.\end{aligned} \tag{39}$$

m, n element of the system density matrix in the interaction picture is

$$\langle m|\tilde{\rho}(t)|n\rangle = e^{i(E_m - E_n)t} \langle m|\hat{\rho}(t)|n\rangle \equiv e^{i(E_m - E_n)t} \rho_{mn}(t), \tag{40}$$

hence the matrix element of its differential is

$$\langle m|\frac{d\tilde{\rho}(t)}{dt}|n\rangle = e^{i(E_m - E_n)t} \Big\{ i(E_m - E_n)\rho_{mn}(t) + \frac{d}{dt}\rho_{mn}(t) \Big\}. \tag{41}$$

Then the final expression of the **master equation** reads

$$\begin{aligned}
\frac{d\rho_{mn}}{dt}\bigg|_{\text{seq.}} &= -i(E_m - E_n)\rho_{mn}(t) \\
+ \sum_\alpha \sum_{pq} \int d\epsilon \frac{\Gamma_\alpha}{2} \Big[f_\alpha(\epsilon) \Big\{ &- \delta(\epsilon - E_p + E_q) \langle m|\hat{d}|p\rangle \langle p|\hat{d}^\dagger|q\rangle \rho_{qn}(t) \\
&- \delta(\epsilon + E_p - E_q)\rho_{mp}(t) \langle p|\hat{d}|q\rangle \langle q|\hat{d}^\dagger|n\rangle \\
&+ (\delta(\epsilon - E_m + E_p) + \delta(\epsilon + E_q - E_n)) \langle m|\hat{d}^\dagger|p\rangle \rho_{pq}(t) \langle q|\hat{d}|n\rangle \Big\} \\
+ \tilde{f}_\alpha(\epsilon) \Big\{ &- \delta(\epsilon - E_p + E_q)\rho_{mp}(t) \langle p|\hat{d}^\dagger|q\rangle \langle q|\hat{d}|n\rangle \\
&+ \delta(\epsilon + E_p - E_q) \langle m|\hat{d}^\dagger|p\rangle \langle p|\hat{d}|q\rangle \rho_{qn}(t) \\
&+ (\delta(\epsilon - E_q + E_n) + \delta(\epsilon + E_m - E_p)) \langle m|\hat{d}|p\rangle \rho_{pq}(t) \langle q|\hat{d}^\dagger|n\rangle \Big\} \Big].
\end{aligned} \tag{42}$$

8.5 GKSL master equation

We are discussing the simplest system, namely, single QD with single level of energy ϵ_0. The only non-zero element of the matrix element $\langle m|\hat{d}|p\rangle$ is for $m = 0$ and $p = 1$ and the matrix element $\langle p|\hat{d}^\dagger|q\rangle$ is for $p = 1$ and $q = 0$. Hence, the master equation can be casted to an operator form

$$\begin{aligned}
\frac{d\hat{\rho}(t)}{dt}\bigg|_{\text{seq.}} &= -i\left[\hat{\mathcal{H}}_{\text{dot}}, \hat{\rho}(t)\right] \\
+ \sum_\alpha \int d\epsilon \frac{\Gamma_\alpha}{2} &\Big[f_\alpha(\epsilon) \Big\{ -\delta(\epsilon - \epsilon_0)\hat{d}\hat{d}^\dagger\hat{\rho}(t) - \delta(\epsilon - \epsilon_0)\hat{\rho}(t)\hat{d}\hat{d}^\dagger + (\delta(\epsilon - \epsilon_0) + \delta(\epsilon - \epsilon_0))\, \hat{d}^\dagger\hat{\rho}(t)\hat{d} \Big\} \\
&+ \tilde{f}_\alpha(\epsilon) \Big\{ -\delta(\epsilon - \epsilon_0)\hat{\rho}(t)\hat{d}^\dagger\hat{d} + \delta(\epsilon - \epsilon_0)\hat{d}^\dagger\hat{d}\hat{\rho}(t) + (\delta(\epsilon - \epsilon_0) + \delta(\epsilon - \epsilon_0))\, \hat{d}\hat{\rho}(t)\hat{d}^\dagger \Big\} \Big] \\
&= -i\left[\hat{\mathcal{H}}_{\text{dot}}, \hat{\rho}(t)\right] \\
&+ \sum_\alpha \Gamma_\alpha f_\alpha(\epsilon_0) \left[\hat{d}^\dagger\hat{\rho}(t)\hat{d} - \frac{1}{2}\Big\{ \hat{d}\hat{d}^\dagger, \hat{\rho}(t) \Big\} \right] + \sum_\alpha \Gamma_\alpha \tilde{f}_\alpha(\epsilon_0) \left[\hat{d}\hat{\rho}(t)\hat{d}^\dagger - \frac{1}{2}\Big\{ \hat{d}^\dagger\hat{d}, \hat{\rho}(t) \Big\} \right],
\end{aligned} \tag{43}$$

where $\Big\{ \hat{d}\hat{d}^\dagger, \hat{\rho}(t) \Big\} = \hat{d}\hat{d}^\dagger\hat{\rho}(t) + \hat{\rho}(t)\hat{d}\hat{d}^\dagger$ is the anti-commutator. This is the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) form of the master equation. [3] In fact, general form of the GKSL master equation is

$$\frac{d\hat{\rho(t)}}{dt} = -i\left[\hat{\mathcal{H}}_{\text{dot}}, \hat{\rho}(t)\right] + \sum_j \gamma_j \left[\hat{L}_j^\dagger\hat{\rho}(t)\hat{L}_j - \frac{1}{2}\Big\{ \hat{L}_j\hat{L}_j^\dagger, \hat{\rho}(t) \Big\} \right], \tag{44}$$

where γ_j is positive constants and $\hat{L}_j$ is system operators, which are called as **jump operators**.

The $(0, 0)$ element of the master equation is

$$\frac{d\rho_{00}(t)}{dt} = -\sum_\alpha \Gamma_\alpha f_\alpha(\epsilon_0)\rho_{00}(t) + \sum_\alpha \Gamma_\alpha \tilde{f}_\alpha(\epsilon_0)\rho_{11}(t), \tag{45}$$

[3] In this simple model, we had proved the microscopic derivation of GKSL master equation from the Redfield equation without further approximations. However, in general cases, we usually need additional condition, *rotating-wave approximation* to achieve GKSL form.

where the first term represents so-called scattering-out and the second term as scattering-in process. Similarly, the element is

$$\frac{d\rho_{11}}{dt} = \sum_{\alpha} \Gamma_\alpha f_\alpha(\epsilon_0)\rho_{00}(t) - \sum_{\alpha} \Gamma_\alpha \tilde{f}_\alpha(\epsilon_0)\rho_{11}(t). \tag{46}$$

These results are identical to those discussed in the previous lectures of the classical master equation.

We also derive the equation for the matrix elements between different $\mathcal{N}$ for the sequential tunneling process. The $(0,1)$ element reads

$$\begin{aligned}\frac{d\rho_{01}}{dt} &= -i(E_0 - E_1)\rho_{01} - \frac{1}{2}\sum_{\alpha} \Gamma_\alpha f_\alpha(E_1 - E_0)\rho_{01} - \frac{1}{2}\sum_{\alpha} \Gamma_\alpha \tilde{f}_\alpha(E_1 - E_0)\rho_{01} \\ &= i\epsilon_0\rho_{01} - \frac{1}{2}\sum_{\alpha} \Gamma_\alpha \rho_{01}.\end{aligned} \tag{47}$$

Hence, the general solution is

$$\rho_{01}(t) = \rho_{01}(0)e^{i\epsilon_0 t - \frac{\Gamma_L + \Gamma_R}{2}t}, \tag{48}$$

whose amplitude exponentially dumps with time. Therefore, we do not need to argue the density matrix elements between different electron number $\mathcal{N}$ since they decay very quickly.

8.6 Expectation of the current

The first order integral-differential equation Eq. (20) can be solved with certain initial condition of $\tilde{\chi}(t)$ as shown in Eq. (20) and we could obtain arbitrary expectation value of an operator $\hat{\mathcal{O}}$,

$$\langle \hat{\mathcal{O}} \rangle (t) \equiv \mathrm{Tr}\left\{\hat{\chi}(t)\hat{\mathcal{O}}\right\} = \mathrm{Tr}\left\{\tilde{\chi}(t)\tilde{\mathcal{O}}(t)\right\}. \tag{49}$$

We are concerning about an electrical current. Using the operator of the total electron density in the reservoir R,

$$\hat{\mathcal{N}}_R = \sum_k \hat{C}^\dagger_{Rk}\hat{C}_{Rk}, \tag{50}$$

the current operator is defined by its change with time:

$$\hat{\mathcal{I}}_R(t) = -e\frac{d}{dt}\hat{\mathcal{N}}_R(t) = -ie[\hat{\mathcal{H}}, \hat{\mathcal{N}}_R(t)] = -ie\sum_k \left\{-V_{Rq}\hat{C}^\dagger_{Rk}(t)\hat{d}(t) + V^*_{Rq}\hat{d}^\dagger_d(t)\hat{C}_{Rk}(t)\right\}. \tag{51}$$

Now the expectation value of the current at time t is obtained using Eq. (20) and noting $\mathrm{Tr}\hat{\chi}_0\hat{I}_R(t) = 0$:

$$I_R(t) = \mathrm{Tr}\left\{\tilde{\chi}(t)\tilde{\mathcal{I}}_R(t)\right\} = -i\int_0^t dt' \mathrm{Tr}\left\{\tilde{\chi}(t')[\tilde{\mathcal{I}}_R(t), \tilde{\mathcal{H}}_1(t')]\right\}, \tag{52}$$

then putting the expression Eq. (51) and $\tilde{\chi}(t') \sim \tilde{\chi}(t) = \hat{R}_0 \otimes \tilde{\rho}(t)$ in the integration kernel, we have the expression for the sequential tunneling current,

$$\begin{aligned} I_R(t) = -e\int_0^\infty d\tau \mathrm{Tr}\Big[\hat{R}_0 \otimes \tilde{\rho}(t)\sum_q\sum_{\alpha k}\Big\{ &- V_{Rq}V^*_{\alpha k}\left[\tilde{C}^\dagger_{Rq}(t)\tilde{d}(t), \tilde{d}^\dagger(t-\tau)\tilde{C}_{\alpha k'}(t-\tau)\right] \\ &+ V^*_{Rq}V_{\alpha k}\left[\tilde{d}^\dagger(t)\tilde{C}_{Rq}(t), \tilde{C}^\dagger_{\alpha k'}(t-\tau)\tilde{d}(t-\tau)\right]\Big\}\Big] \\ = ie\sum_{mpq}\rho_{qm}(t)\int\frac{d\epsilon}{2\pi}\Gamma_R\Big[&- f_R(\epsilon)\left\{-2\pi i\delta(\epsilon-\epsilon_0)\right\}\langle m|\hat{d}|p\rangle\langle p|\hat{d}^\dagger|q\rangle \\ &+ \tilde{f}_R(\epsilon)\left\{-2\pi i\delta(\epsilon-\epsilon_0)\right\}\langle m|\hat{d}^\dagger|p\rangle\langle p|\hat{d}|q\rangle\Big]. \end{aligned} \tag{53}$$

Now we can obtain the current with this expression after solving the differential equation Eq. (42). The current expectation value is determined with using the solution of Eq. (45)[2] :

$$I_R(t) = e\Gamma_R f_R(E)\rho_{00}(t) - e\Gamma_R\tilde{f}_R(E)\rho_{11}(t). \tag{54}$$

8.7 Conclusions

We have obtained the master equation and the sequential current expression for a quantum dot (QD) coupled with two reservoirs. The formula is applied to the problems of single-QD with single level. This formalism can be extended to the system of multi-levels in a QD or multiple QDs and the system with Coulomb interaction between the occupied electrons[3]. However, it should be stressed here that the Born-Markov approximation applied to this simple model corresponds to the situation that the quantum dot is weakly coupled to the reservoirs and there is rapid decoherencing process for the electron occupying the quantum dot. Therefore, this formalism cannot account for the coherent transport through the system like resonant tunneling process. I would like to touch this issue in the last part of this lecture.

References

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