Quantum theory of condensed matter II

Mesoscopic physics (Quantum transport)

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Sheet 13

1. Master equation for the Anderson impurity model

Let us consider an Anderson impurity coupled to an electronic lead. We model such an open system using the following Hamiltonian

$$\hat{H} = \hat{H}_{\mathrm{S}} + \hat{H}_{\mathrm{B}} + \hat{H}_{\mathrm{T}}$$

where

$$\hat{H}_{\mathrm{S}} = \sum_{\sigma} \varepsilon_d \, \hat{d}_\sigma^\dagger \hat{d}_\sigma + U \hat{n}_\uparrow \hat{n}_\downarrow, \tag{1a}$$

$$\hat{H}_{\mathrm{B}} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \, \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma}, \tag{1b}$$

$$\hat{H}_{\mathrm{T}} = \sum_{\mathbf{k}\sigma} \tau \left(\hat{c}_{\mathbf{k}\sigma}^\dagger \hat{d}_\sigma + \hat{d}_\sigma^\dagger \hat{c}_{\mathbf{k}\sigma} \right). \tag{1c}$$

The Hamiltonian $\hat{H}_{\mathrm{S}}$ describes the Anderson impurity: $\hat{d}_\sigma^\dagger$ creates an electron with spin σ and spin independent energy ε_{d}, $\hat{n}_\sigma = \hat{d}_\sigma^\dagger \hat{d}_\sigma$ counts the number of electrons with spin σ on the impurity, U is the strength of the electron-electron interaction on the impurity site. $\hat{H}_{\mathrm{B}}$ is the Hamiltonian of non interacting electrons with dispersion relation $\varepsilon_{\mathbf{k}}$ and wave number $\mathbf{k}$. Moreover $\hat{H}_{\mathrm{T}}$ accounts for the tunneling processes between the impurity and the bath. For simplicity let us assume real, spin and momentum independent tunneling matrix elements τ. Let us study the dynamics of the system by means of the reduced density matrix. Let us assume that the full density matrix can be written in a factorized form $\hat{\rho}(t=0) = \hat{\rho}_{\mathrm{S}}(0) \otimes \hat{\rho}_{\mathrm{B}}(0)$ at time $t = 0$ and that $\hat{\rho}_{\mathrm{B}}(0)$ is described by the gran-canonical distribution $\hat{\rho}_{\mathrm{B}}(0) = e^{-\beta\left(\hat{H}_{\mathrm{B}} - \mu \hat{N}_{\mathrm{B}}\right)}/\mathcal{Z}$ where $\mathcal{Z} = \mathsf{Tr}_{\mathrm{B}} \left\{ e^{-\beta\left(\hat{H}_{\mathrm{B}} - \mu \hat{N}_{\mathrm{B}}\right)} \right\}$ is the partition function, μ is the chemical potential, β the inverse of the thermal energy and $\hat{N}_{\mathrm{B}}$ the bath's number operator.

1. By following the same steps introduced in Sheet 7 for the spin boson model, prove that the reduced density matrix fulfills the following equation in the interaction picture, valid up to second order in the tunneling matrix element τ:
$$\dot{\hat{\rho}}_{\mathrm{red,\,I}}(t) = -\frac{1}{\hbar^2} \int_0^t \mathrm{d}t' \, \mathsf{Tr}_{\mathrm{B}} \left\{ \left[\hat{H}_{\mathrm{T,I}}(t), \left[\hat{H}_{\mathrm{T,I}}(t'), \hat{\rho}_{\mathrm{red,I}}(t') \otimes \hat{\rho}_{\mathrm{B}}(0) \right] \right] \right\} \tag{2}$$
where $\hat{\rho}_{\mathrm{red,I}}(t) = \mathsf{Tr}_{\mathrm{B}} \left\{ \hat{\rho}_{\mathrm{I}}(t) \right\}$. **(1 Point)**
2. By using the explicit form of the tunnelling Hamiltonian and the bath density matrix, show that Eq. (2) may

be written in the form:

$$
\begin{aligned}
\dot{\hat{\rho}}_{\mathrm{red,I}}(t) = -\frac{\tau^2}{\hbar^2}\sum_\sigma \int_0^t \mathrm{d}t' \, [\quad & F(t-t',+\mu)\, \hat{d}_\sigma(t)\hat{d}^\dagger_\sigma(t')\, \hat{\rho}_{\mathrm{red,I}}(t') \\
& + F(t-t',-\mu)\, \hat{d}^\dagger_\sigma(t)\hat{d}_\sigma(t')\, \hat{\rho}_{\mathrm{red,I}}(t') \\
& - F^*(t-t',-\mu)\, \hat{d}_\sigma(t)\hat{\rho}_{\mathrm{red,I}}(t')\hat{d}^\dagger_\sigma(t') \\
& - F^*(t-t',+\mu)\, \hat{d}^\dagger_\sigma(t)\, \hat{\rho}_{\mathrm{red,I}}(t')\hat{d}_\sigma(t') \\
& + \mathrm{h.c.}].
\end{aligned}
\tag{3}
$$

where the correlator $F(t-t',\mu)$ is defined as:

$$
F(t-t',\mu) = \sum_{\mathbf{k}} \mathsf{Tr}_{\mathrm{B}}\left\{\hat{c}^\dagger_{\mathbf{k}\sigma}(t)\hat{c}_{\mathbf{k}\sigma}(t')\hat{\rho}_{\mathrm{B}}\right\}
$$

and all the operators, including the density operators, are in interaction picture. **(2 Points)**

3. Let us evaluate $F(t-t',\mu)$. To this extent let us evaluate the sum with respect to the wave number $\mathbf{k}$ as

$$
\sum_{\mathbf{k}} g(\mathbf{k}) = \int_{-\infty}^{+\infty} \mathrm{d}\varepsilon L(\varepsilon-\mu,W)g(\varepsilon),
$$

where we introduced the density of states (DOS) $L(\varepsilon-\mu,W) = \sum_{\mathbf{k}} \delta(\varepsilon-\mu-\varepsilon_{\mathbf{k}})$. In the following, since we are not interested in the effects due to a specific form of the DOS, let us assume a Lorentzian density of states in the electronic bath

$$
L(\varepsilon-\mu,W) = D_0\frac{W^2}{(\varepsilon-\mu)^2+W^2},
$$

where W is the bandwidth and D_0 is the density of states at the Fermi level. Prove that $F(t-t',\mu)$, in the wide bandwidth ($W \gg \beta^{-1}, \varepsilon_{\mathrm{d}}, U, \tau$) and in the long time $W(t-t')/\hbar \gg 1$ limits, may be approximated as

$$
F(t-t',\mu) \simeq -\pi\frac{D_0}{\beta}\, e^{\frac{i}{\hbar}\mu(t-t')}\frac{i}{\sinh\left(\pi\frac{t-t'}{\hbar\beta}\right)}.
$$

Hint: Use the Residuum theorem to compute the following integration

$$
\int_{-\infty}^{+\infty} \mathrm{d}\varepsilon\, L(\varepsilon,W)f(\varepsilon)e^{i\frac{\varepsilon}{\hbar}(t-t')} =
$$

$$
\frac{D_0}{\beta}2\pi i\left[\sum_{k=0}^{+\infty}\frac{-W^2}{W^2-\left[(2k+1)\pi\beta^{-1}\right]^2}e^{-\frac{(2k+1)\pi}{\hbar\beta}(t-t')} - i\frac{W\beta}{2\left(1+e^{i\beta W}\right)}e^{-\frac{W}{\hbar}(t-t')}\right],
$$

where $f(\varepsilon) = 1/(1+\exp(\beta\varepsilon))$ is the Fermi function. Then consider the wide bandwidth $W/\beta^{-1} \gg 1$ and the long time $W(t-t')/\hbar \gg 1$ limits up to the zeroth order in the corresponding analytic terms.

(4 Points)

4. The correlator $F(t-t',\mu)$ decays with respect to the time difference $t-t'$ approximately as $\exp(-\pi\frac{t-t'}{\hbar\beta})$. Prove that the variation rate of the density matrix is of the order $\gamma = \frac{2\pi\tau^2 D_0}{\hbar}$. Finally, discuss, similarly to the spin boson model, the validity of the Markov approximation. I.e. i) local time approximation, *i.e.* $t' \to t$ in the argument of the reduced density matrix inside the time integral in the limit $\hbar\gamma \ll k_{\mathrm{B}}T$; ii) If we are interested into a time dynamics on time scales larger than the bath correlation time $\hbar\beta$, the time integration limit can be moved from the initial time $t_0 = 0$ to $t_0 = -\infty$. **(2 Points)**

5. Transform the equation from the interaction to the Schrödinger picture:

$$\dot{\hat{\rho}}_{\text{red}}(t) = -\frac{i}{\hbar}\left[\hat{H}_{\text{S}}, \hat{\rho}_{\text{red}}(t)\right] - \frac{\tau^2}{\hbar^2}\sum_{\sigma}\int\limits_0^{\infty} \mathrm{d}t' \Big[\quad F(t', +\mu)\, \hat{d}_{\sigma}\hat{d}^{\dagger}_{\sigma}(-t')\, \hat{\rho}_{\text{red}}(t)$$
$$+ F(t', -\mu)\, \hat{d}^{\dagger}_{\sigma}\hat{d}_{\sigma}(-t')\, \hat{\rho}_{\text{red}}(t)$$
$$- F^*(t', -\mu)\, \hat{d}_{\sigma}\hat{\rho}_{\text{red}}(t)\hat{d}^{\dagger}_{\sigma}(-t')$$
$$- F^*(t', +\mu)\, \hat{d}^{\dagger}_{\sigma}\, \hat{\rho}_{\text{red}}(t)\hat{d}_{\sigma}(-t')$$
$$+ \text{h.c.}\Big]. \tag{4}$$

where the density operators are in the Schrödinger picture, while the creation and annihilation operators of the impurity are still in the interaction picture.

6. Find the eigenenergies of the impurity system and write the equations for the populations in that basis using Eq.(4).

7. Considering the analytic expression of the correlator $F(t-t', \mu)$ that you have calculated in point 13.2, perform the time integral in Eq.(4) and obtain the master equation for the populations:

$$\dot{P}_0(t) = -2\gamma L\left(\varepsilon_{\text{d}} - \mu, W\right) f^+(\varepsilon_{\text{d}}) P_0(t) + \gamma L\left(\varepsilon_{\text{d}} - \mu, W\right) \sum_{\sigma} f^-(\varepsilon_{\text{d}}) P_{1\sigma}(t) \tag{5a}$$

$$\begin{aligned}\dot{P}_{1\sigma}(t) = {} & \gamma L(\varepsilon_{\text{d}} - \mu, W) f^+\left(\varepsilon_{\text{d}}\right) P_0(t) + \\ & - \gamma \left[L\left(\varepsilon_{\text{d}} + U - \mu, W\right) f^+\left(\varepsilon_{\text{d}} + U\right) + L\left(\varepsilon_{\text{d}} - \mu, W\right) f^-\left(\varepsilon_{\text{d}}\right)\right] P_{1\sigma}(t) + \\ & + \gamma L\left(\varepsilon_{\text{d}} + U - \mu, W\right) f^-\left(\varepsilon_{\text{d}} + U\right) P_2(t)\end{aligned} \tag{5b}$$

$$\dot{P}_2(t) = +\gamma \sum_{\sigma} L\left(\varepsilon_{\text{d}} + U - \mu, W\right) f^+\left(\varepsilon_{\text{d}} + U\right) P_{1\sigma}(t) - 2\gamma L\left(\varepsilon_{\text{d}} + U - \mu, W\right) f^-\left(\varepsilon_{\text{d}} + U\right) P_2(t) \tag{5c}$$

where $P_0(t) \equiv \langle 0|\hat{\rho}_{\text{red}}(t)|0\rangle$, $P_{1\sigma} \equiv \langle 1\sigma|\hat{\rho}_{\text{red}}(t)|1\sigma\rangle$ and $P_2(t) \equiv \langle 2|\hat{\rho}_{\text{red}}(t)|2\rangle$ are the populations of the reduced density matrix with respect to the energy eigenbasis $|0\rangle, |1\uparrow\rangle, |1\downarrow\rangle, |2\rangle$ of the impurity. Moreover $f^+(\epsilon) \equiv [1+\exp(\beta(\epsilon-\mu))]^{-1}$ and $f^-(\epsilon) \equiv f^+(-\epsilon)$.
In the stationary limit $\dot{P}_i = 0$ for $i \in \{\ |0\rangle,\ |1\sigma\rangle,\ |2\rangle\ \}$. Is the linear system of equations well defined? What is the physical interpretation? How do we solve this issue?

Hint: Perform the integration with respect to the time difference $t - t'$ of the exponential dependence in $F(t-t', \mu)$ keeping into account that

$$2\text{Re}\int_0^{\infty} \mathrm{d}t F(t, \mu) e^{i\frac{\varepsilon_{\text{d}}}{\hbar}} = 2\pi\hbar L(\varepsilon_{\text{d}} - \mu, W) f^+(\varepsilon_{\text{d}}).$$

8. Prove that the stationary solution of the master equation is:

 i) $P_0 = 1$, $P_{1\sigma} = P_2 = 0$ for $\mu \ll \varepsilon_{\text{d}}$;

 ii) $P_2 = 1$, $P_{1\sigma} = P_0 = 0$ for $\mu \gg \varepsilon_{\text{d}} + U$;

 iii) $P_{1\sigma} = 1/2$, $P_2 = P_0 = 0$ for $\varepsilon_{\text{d}} \ll \mu \ll \varepsilon_{\text{d}} + U$;

 where inequalities are taken with respect to the thermal energy $k_{\text{B}}T$ and the solution iii) is considered in the limit $U \gg k_{\text{B}}T$. Comment the result.

Frohes Schaffen!