

Density Matrix Theory

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Sheet 4

1. Master equation for the Anderson impurity model (I)

Consider an (Anderson) impurity coupled by tunneling to an electronic reservoir. This open system can be described by the Hamiltonian

$$H = H_S + H_B + H_T$$

where

$$\begin{aligned} H_S &= \sum_{\sigma} \varepsilon_d d_{\sigma}^{\dagger} d_{\sigma} + U n_{\uparrow} n_{\downarrow}, \\ H_B &= \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma}, \\ H_T &= \sum_{\mathbf{k}\sigma} \tau \left(c_{\mathbf{k}\sigma}^{\dagger} d_{\sigma} + d_{\sigma}^{\dagger} c_{\mathbf{k}\sigma} \right). \end{aligned}$$

The Hamiltonian H_S describes the Anderson impurity: d_{σ}^{\dagger} creates an electron with spin σ and spin independent energy ε_d ; the operator $n_{\sigma} = d_{\sigma}^{\dagger} d_{\sigma}$ counts the number of electrons with spin σ on the impurity; the interaction energy U must be paid to have two electrons on the impurity. With H_B we represent a bath of non interacting electrons with dispersion relation $\varepsilon_{\mathbf{k}}$. Finally H_T accounts for the tunneling processes between the impurity and the bath. For simplicity we assume that the tunneling amplitude τ is real and independent of the spin and the momentum $\hbar\mathbf{k}$ of the bath state. We want to calculate the dynamics of the system in terms of the reduced density matrix.

1. Assume that at time $t = 0$ the full density matrix can be written in a factorized form $\rho(0) = \rho_S(0) \otimes \rho_B(0)$ and assume for $\rho_B(0)$ the grandcanonical distribution $\rho_B(0) = \frac{1}{\mathcal{Z}} e^{-\beta(H_B - \mu N_B)}$ where $\mathcal{Z} = \text{Tr}_B \{ e^{-\beta(H_B - \mu N_B)} \}$ is the partition function, μ is the chemical potential, β the inverse of the thermal energy and N_B the bath number operator.

Prove the following relation for the density matrix at time t :

$$\rho_I(t) = \text{Tr}\{\rho_I(t)\} \otimes \rho_B + O(H_T)$$

where the index I indicates the interaction picture, taking H_T as the perturbation. Hint: remember that vectors evolve in the interaction picture as:

$$|\psi(t)\rangle_I = U_I(t, 0) |\psi(0)\rangle_I$$

where

$$U_I(t, 0) = T_{\leftarrow} \exp \left[-\frac{i}{\hbar} \int_0^t dt' H_{T,I}(t') \right]$$

with the usual time ordering.

2. Using the result obtained in the previous point derive the following equation of motion for the reduced density matrix, valid up to second order in the tunneling Hamiltonian H_T :

$$\dot{\rho}_{red,I}(t) = -\frac{1}{\hbar^2} \int_0^t dt' \text{Tr}_B \{ [H_{T,I}(t), [H_{T,I}(t'), \rho_{red,I}(t') \otimes \rho_B(0)]] \} \quad (1)$$

where $\rho_{red,I}(t) = \text{Tr}\{\rho_I(t)\}$.

3. By inserting explicitly the form of the tunneling hamiltonian and the bath density matrix show that, for a bath with a constant density of states over the entire energy range, (wide band limit) Eq. (1) can be written in the form:

$$\begin{aligned} \dot{\rho}_{red}(t) = & -\frac{\tau^2}{\hbar^2} \sum_{\sigma} \int_0^t dt' [+F(t-t', +\mu) d_{\sigma}(t) d_{\sigma}^{\dagger}(t') \rho_{red}(t') \\ & + F(t-t', -\mu) d_{\sigma}^{\dagger}(t) d_{\sigma}(t') \rho_{red}(t') \\ & - F^*(t-t', -\mu) d_{\sigma}(t) \rho_{red}(t') d_{\sigma}^{\dagger}(t') \\ & - F^*(t-t', +\mu) d_{\sigma}^{\dagger}(t) \rho_{red}(t') d_{\sigma}(t') \\ & + \text{Hermitian conjugate}]. \end{aligned} \quad (2)$$

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

$$F(t-t', \mu) = \sum_{\mathbf{k}} \text{Tr}_B \{ c_{\mathbf{k}\sigma}^{\dagger}(t) c_{\mathbf{k}\sigma}(t') \rho_B \}$$

and all the operators, including the density operators, are taken in interaction picture.

4. Prove that $F(t-t', \mu)$ has, in the wide band limit, the following form:

$$F(t-t', \mu) = \pi \hbar D e^{\frac{i}{\hbar} \mu(t-t')} \left[\delta(t-t') - \frac{i}{\hbar \beta \sinh(\pi \frac{t-t'}{\hbar \beta})} \right]$$

where D is the (constant) density of states of the bath.

Hint: The following integral can be useful for the calculation:

$$\int_0^{\infty} dx \sin(ax) \tanh\left(\frac{bx}{2}\right) = \frac{\pi}{b \sinh\left(\frac{\pi a}{b}\right)}$$

for a and $b \in \mathbb{R}$.

5. You just proved that the correlator $F(t-t', \mu)$ decays with the time difference $t-t'$ approximately as $\exp(-\pi \frac{t-t'}{\hbar \beta})$. Prove that the rate of variation of the density matrix is of the order $\gamma = \frac{2\pi \tau^2 D}{\hbar}$. Finally justify the validity of the local time approximation, *i.e.* $t' \rightarrow t$ (first step of the Markov) in the argument of the reduced density matrix inside the time integral, in the limit $\hbar \gamma \ll k_B T$.

Frohes Schaffen!