Density Matrix Theory

Lectures	Tue	12:00 - 13:30	PHY 5.0.20
	Thu	10:15 - 12:00	PHY 9.1.09
Exercises	Fri	10:15 - 12:00	PHY 5.0.21

Sheet 4

1. Master equation for the Anderson impurity model

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

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

where

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

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

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

The Hamiltonian $\hat{\mathrm{H}}_{\mathrm{S}}$ describes the Anderson impurity: $\hat{\mathrm{d}}^\dagger_\sigma$ creates an electron with spin σ and spin independent energy ε_{d}, $\hat{\mathrm{n}}_\sigma = \hat{\mathrm{d}}^\dagger_\sigma \hat{\mathrm{d}}_\sigma$ counts the number of electrons with spin σ on the impurity, U is the strength of the electron-electron interaction on the impurity site. $\hat{\mathrm{H}}_{\mathrm{B}}$ is the Hamiltonian of non interacting electrons with dispersion relation $\varepsilon_{\mathbf{k}}$ and wave number $\mathbf{k}$. Moreover $\hat{\mathrm{H}}_{\mathrm{T}}$ 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 $\hat{\rho}_{\mathrm{B}}(0) = e^{-\beta\left(\hat{\mathrm{H}}_{\mathrm{B}} - \mu \hat{\mathrm{N}}_{\mathrm{B}}\right)}/\mathcal{Z}$ where $\mathcal{Z} = \mathsf{Tr}_{\mathrm{B}}\left\{ e^{-\beta\left(\hat{\mathrm{H}}_{\mathrm{B}} - \mu \hat{\mathrm{N}}_{\mathrm{B}}\right)} \right\}$ is the partition function, μ is the chemical potential, β the inverse of the thermal energy and $\hat{\mathrm{N}}_{\mathrm{B}}$ the bath's number operator.

Then, as it was shown in the lecture, the reduced density matrix fulfills the following equation in the interaction picture, valid up to second order in the tunneling matrix element τ:

$$\dot{\hat{\rho}}_{\mathrm{red,\,I}}(t) = -\frac{1}{\hbar^2} \int_0^t \mathrm{d}t' \, \mathsf{Tr}_{\mathrm{B}} \left\{ \left[\hat{\mathrm{H}}_{\mathrm{T,I}}(t), \left[\hat{\mathrm{H}}_{\mathrm{T,I}}(t'), \hat{\rho}_{\mathrm{red,I}}(t') \otimes \hat{\rho}_{\mathrm{B}}(0) \right] \right] \right\} \tag{2}$$

where $\hat{\rho}_{\mathrm{red,I}}(t) = \mathsf{Tr}_{\mathrm{B}}\left\{ \hat{\rho}_{\mathrm{I}}(t) \right\}$.

1. Using the explicit form of the tunneling Hamiltonian and the bath density matrix, show that Eq. (2) may be written in the form:

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

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. 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) $L(\varepsilon-\mu,W) = \sum_{\mathbf{k}} \delta\left(\varepsilon-\mu-\varepsilon_{\mathbf{k}}\right)$. 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

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

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.

3. 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 the validity of the local time approximation, *i.e.* $t' \to t$ in the argument of the reduced density matrix inside the time integral (*Markov approximation*), in the limit $\hbar\gamma \ll k_{\mathrm{B}}T$.

Frohes Schaffen!