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 5

1. Markovian master equation for the Anderson impurity model

Let us consider an Anderson impurity coupled to an electronic lead as in Sheet 4

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

where

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

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

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

Assuming the high temperature limit ($k_{\mathrm{B}}T \gg \hbar\gamma$ where $\gamma = \frac{2\pi\tau^2 D_0}{\hbar}$ and D_0 is the the bath density of states at the Fermi level) we derived the following time local equation for the reduced density matrix, valid up to second order in the tunnelling Hamiltonian H_{T},

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

where all the operators are in the interaction picture and the bath correlation function is defined as

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

Following the same arguments given in the lecture one can argue that, 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 $t_0 = -\infty$ (Markov approximation). A transformation to the Schrödinger picture yields:

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

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

1. Find the eigenenergies of the impurity system and write the equations for the populations in that basis using Eq.(3).

2. Considering the analytic expression of the correlator $F(t-t',\mu)$ we have found in Sheet 4, perform the time integral in Eq.(3) and obtain the master equation for the populations:

$$\dot{P}_0(t) = -2\gamma L\left(\varepsilon_\mathrm{d}-\mu,W\right)f^+(\varepsilon_\mathrm{d})P_0(t) + \gamma L\left(\varepsilon_\mathrm{d}-\mu,W\right)\sum_\sigma f^-(\varepsilon_\mathrm{d})P_{1\sigma}(t) \tag{4a}$$

$$\begin{aligned}\dot{P}_{1\sigma}(t) = {} & \gamma L(\varepsilon_\mathrm{d}-\mu,W)f^+\left(\varepsilon_\mathrm{d}\right)P_0(t) + \\ & -\gamma\left[L\left(\varepsilon_\mathrm{d}+U-\mu,W\right)f^+\left(\varepsilon_\mathrm{d}+U\right) + L\left(\varepsilon_\mathrm{d}-\mu,W\right)f^-\left(\varepsilon_\mathrm{d}\right)\right]P_{1\sigma}(t) + \\ & +\gamma L\left(\varepsilon_\mathrm{d}+U-\mu,W\right)f^-\left(\varepsilon_\mathrm{d}+U\right)P_2(t)\end{aligned} \tag{4b}$$

$$\dot{P}_2(t) = +\gamma\sum_\sigma L\left(\varepsilon_\mathrm{d}+U-\mu,W\right)f^+\left(\varepsilon_\mathrm{d}+U\right)P_{1\sigma}(t) - 2\gamma L\left(\varepsilon_\mathrm{d}+U-\mu,W\right)f^-\left(\varepsilon_\mathrm{d}+U\right)P_2(t) \tag{4c}$$

where $P_0(t) \equiv \langle 0|\hat{\rho}_\mathrm{red}(t)|0\rangle$, $P_{1\sigma} \equiv \langle 1\sigma|\hat{\rho}_\mathrm{red}(t)|1\sigma\rangle$ and $P_2(t) \equiv \langle 2|\hat{\rho}_\mathrm{red}(t)|2\rangle$ 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

$$\int_0^{+\infty} \mathrm{d}x\, e^{-ax}e^{-ibx} = \frac{1}{a+ib} \quad \text{with } a>0, b\in\mathbb{R}.$$

Moreover after the integration the following identity may be useful in order to sum the series

$$\sum_{k=0}^{\infty} \frac{x}{\left[(2k+1)\pi\right]^2 + x^2}\frac{y^2}{y^2-\left[(2k+1)\pi\right]^2} = \frac{1}{4}\left[\frac{y^2}{y^2+x^2}\tanh\left(\frac{x}{2}\right) - \frac{xy}{y^2+x^2}\tan\left(\frac{y}{2}\right)\right]$$

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

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

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

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

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

Frohes Schaffen!