Universität Regensburg Wintersemester 13-14

Density Matrix Theory

Prof. Andrea Donarini 5.0.21, Tuesdays, 10:15

Sheet 5

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

Let us continue in the derivation of the master equation for the Hamiltonian introduced in the Sheet 4, namely:

$$H = H_{\rm S} + H_{\rm B} + H_{\rm T}$$

where

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

By assuming the high temperature limit ($k_{\rm B}T \gg \hbar\gamma$ where $\gamma = \frac{\pi\tau^2 D}{\hbar}$ and D is the density of states of the bath) we derived the following time local equation for the reduced density matrix, valid to second order in the tunnelling Hamiltonian $H_{\rm T}$:

$$\begin{aligned} \dot{\rho}_{red}(t) = -\frac{\tau^2}{\hbar^2} \sum_\sigma \int_0^t {\rm d}t' [&+F(t-t',+\mu)\, d_\sigma(t) d^\dagger_\sigma(t')\, \rho_{red}(t) \\ &+ F(t-t',-\mu)\, d^\dagger_\sigma(t) d_\sigma(t')\, \rho_{red}(t) \\ &- F^*(t-t',-\mu)\, d_\sigma(t) \rho_{red}(t) d^\dagger_\sigma(t') \\ &- F^*(t-t',+\mu)\, d^\dagger_\sigma(t)\, \rho_{red}(t) d_\sigma(t') \\ &+ \text{Hermitian conjugate}]. \end{aligned} \tag{1}$$

where all operators are taken in interaction picture and the bath correlation function $F(t-t',\mu)$ is defined as

$$F(t-t',\mu) = \sum_{\mathbf{k}} {\rm Tr}_{\rm B}\{ c^\dagger_{\mathbf{k}\sigma}(t) c_{\mathbf{k}\sigma}(t') \rho_{\rm B} \}$$

1. Argue that, if we are interested into a time dynamics on time scales larger than the bath correlation time $\hbar\beta$ (the so called coarse grained limit) the time integration limit can be moved from the initial time $t_0 = 0$ to $t_0 = -\infty$ (Markoff approximation).

2. Transform the equation from the interaction to the Schrödinger picture. Prove that the result will be:

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

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

3. In the calculation of the time evolution for isolated system we have already demonstrated that it is extremely useful for the understanding of the dynamics to write the equations in the energy eigenbasis for the system. Calculate the energy eigenbasis for the impurity and write Eq.(2) in that basis.

4. Prove that the dynamics of the spin coherences (matrix elements corresponding to different spin projection S_z of the system) is decoupled from the dynamics of the corresponding populations.

5. Prove that the same decoupling is happening between coherences involving different particle number and the corresponding populations. Could you imagine a bath for which this decoupling is violated? Why?

6. Prove that the coherent term (the first term in Eq.(2)) does not influence the dynamics of the populations in the energy eigenbasis.

7. Perform the time integral in Eq. (2) and get to the master equation for populations:

$$
\begin{aligned}
\dot{P}_0 = & -2\gamma f^+(\varepsilon_d)P_0 + \gamma\sum_\sigma f^-(\varepsilon_d)P_{1\sigma} \\
\dot{P}_{1\sigma} = & -\gamma[f^+(\varepsilon_d+U) + f^-(\varepsilon_d)]P_{1\sigma} \\
& + \gamma f^+(\varepsilon_d)P_0 + \gamma f^-(\varepsilon_d+U)P_2 \\
\dot{P}_2 = & -2\gamma f^-(\varepsilon_d+U)]P_2 + \gamma\sum_\sigma f^+(\varepsilon_d+U)P_{1\sigma}
\end{aligned}
$$

where

$$
P_0(t) \equiv \langle 0|\rho_{red}(t)|0\rangle P_{1\sigma} \equiv \langle 1\sigma|\rho_{red}(t)|1\sigma\rangle P_2(t) \equiv \langle 2|\rho_{red}(t)|2\rangle
$$

are the populations of the reduced density matrix with respect to the manybody energy eigenbasis $|0\rangle$, $|1\uparrow\rangle$, $|1\downarrow\rangle$, $|2\rangle$ of the impurity. Moreover $f^+(\epsilon) \equiv [1+e^{\beta(\epsilon-\mu)}]^{-1}$ and $f^-(\epsilon) \equiv 1 - f^+(\epsilon)$.

8. Prove that the stationary solution of the master equation derived in the previous point is:

$$
\begin{aligned}
\text{i)} \quad & P_0 = 1,\ P_{1\sigma} = P_2 = 0 \quad \text{for} \quad \mu \ll \varepsilon_d; \\
\text{ii)} \quad & P_2 = 1,\ P_{1\sigma} = P_0 = 0 \quad \text{for} \quad \mu \gg \varepsilon_d + U; \\
\text{iii)} \quad & P_{1\sigma} = 1/2,\ P_0 = P_2 = 0 \quad \text{for} \quad \varepsilon_d \ll \mu \ll \varepsilon_d + U.
\end{aligned}
$$

where inequalities are taken with respect to the thermal energy $k_\mathrm{B}T$ and the solution iii) can thus be achieved only in the case $U \gg k_\mathrm{B}T$. Comment the result.

Frohes Schaffen!