Density Matrix Theory

Lectures	Wed	11:15 - 12:45	PHY 2.0.31
	Thu	10:00 - 11:30	PHY 2.1.29
Exercises	Fri	14:00 - 15:45	PHY 9.1.10

Sheet 6

1. Equilibrium: the free energy formulation

Consider the master equation for the Anderson impurity model introduced in the Sheet 4:

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

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.

1. Prove that the stationary solution of this master equation is independent of the magnitude of the bare tunnelling rate γ and, for every value of the parameters (ε_d, U, μ, T) defining the model, can be written in the form:

$$\begin{aligned}P_0^{stat} &= \frac{1}{N}f^-(\varepsilon_d)f^-(\varepsilon_d+U)\\ P_{1\sigma}^{stat} &= \frac{1}{N}f^+(\varepsilon_d)f^-(\varepsilon_d+U)\\ P_2^{stat} &= \frac{1}{N}f^+(\varepsilon_d)f^+(\varepsilon_d+U)\end{aligned} \tag{1}$$

   where N is the normalization factor that ensures the sum of the probability to be 1. Moreover $f^+(\epsilon) \equiv [1+e^{\beta(\epsilon-\mu)}]^{-1}$ and $f^-(\epsilon) \equiv 1 - f^+(\epsilon)$.

2. Prove that the equilibrium probabilities derived at the previous point can be obtained from a thermodynamical formulation of the problem where the impurity, defined by the Hamiltonian H_S (see Sheet 4), can exchange energy and particles with a bath with temperature T and chemical potential μ. In particular calculate the grand canonical partition function $\mathcal{Z} = \mathrm{Tr_S}\{e^{-\beta(H_\mathrm{S}-\mu N_\mathrm{S})}\}$ for the impurity and prove that:

$$P_\alpha^{stat} = \frac{1}{\mathcal{Z}}\mathrm{Tr_S}\{|\alpha\rangle\langle\alpha|e^{-\beta(H_\mathrm{S}-\mu N_\mathrm{S})}\}$$

   where $|\alpha\rangle$ is a manybody energy eigenstate of the impurity and N_S the particle number.

Frohes Schaffen!