Density Matrix Theory

Prof. Andrea Donarini 5.0.21, Tuesdays, 10:15

Sheet 6

1. Equilibrium: the free energy formulation

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

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

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 $H_{\rm S}$ (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 $\mathcal{Z} = {\rm Tr_S}\{e^{-\beta(H_{\rm S}-\mu N_{\rm S})}\}$ for the impurity and prove that:

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

   where $|\alpha\rangle$ is a manybody energy eigenstate of the impurity and $N_{\rm S}$ the particle number.

2. Time evolution for a Markovian master equation

In this exercise we consider the Markoff master equation (1) and calculate numerically the time evolution for the populations of the many-body states of the impurity.

1. Show that the equations (1) can be cast into a matrix form $\dot{P}(t) = LP(t)$ where $P \equiv (P_0, P_{1\uparrow}, P_{1\downarrow}, P_2)^T$ and

$$L = \gamma \begin{pmatrix} -2f^+(\varepsilon_d) & f^-(\varepsilon_d) & f^-(\varepsilon_d) & 0 \\ f^+(\varepsilon_d) & -f^-(\varepsilon_d) - f^+(\varepsilon_d + U) & 0 & f^-(\varepsilon_d + U) \\ f^+(\varepsilon_d) & 0 & -f^-(\varepsilon_d) - f^+(\varepsilon_d + U) & f^-(\varepsilon_d + U) \\ 0 & f^+(\varepsilon_d + U) & f^+(\varepsilon_d + U) & -2f^-(\varepsilon_d + U) \end{pmatrix}.$$

   Prove that the solution of the equation can be written in the form $P(t) = e^{Lt}P(t = 0)$. Taking advantage of this algebraic formulation, calculate the numerical solution of (1). Hint: the function "expm" calculates the exponential of a matrix in Matlab.

2. Prove that, if the time is measured in units of $1/\gamma$ solutions with different tunneling rates coincide.

3. Check that the stationary solution is reached by the system after a time corresponding to a few $1/\gamma$ and that it is independent of the initial condition.

4. Calculate the time evolution for the population vector P also with the help of one of the packages for ordinary differential equations available in Matlab. Compare the results with the previous method. Hint: There are different types of solvers. You can start by typing "help ode23" in the command line and read the documentation.

Frohes Schaffen!