

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 7

1. The Anderson impurity model with multiple baths

Let us consider again the Anderson impurity introduced in the Sheet 4 but this time in tunneling contact with a set of baths. While the system Hamiltonian remains unchanged, the bath and tunneling Hamiltonians read:

$$H_B = \sum_{\alpha\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\alpha\mathbf{k}\sigma}^\dagger c_{\alpha\mathbf{k}\sigma},$$

$$H_T = \sum_{\alpha\mathbf{k}\sigma} \tau_\alpha \left(c_{\alpha\mathbf{k}\sigma}^\dagger d_\sigma + d_\sigma^\dagger c_{\alpha\mathbf{k}\sigma} \right),$$

respectively. With α we label the different baths and for simplicity we assume the same dispersion relation for the different baths. The tunnelling coupling τ_α is, instead, different to the different baths and we also assume a different equilibrium temperature T_α and chemical potential μ_α for each of the baths.

1. Assume that: i) The tunnelling Hamiltonian H_T can be treated perturbatively; ii) The impurity and the baths are uncorrelated at time $t = 0$ (*i.e.* $\rho = \rho_S \otimes \rho_B$). iii) The baths are not correlated between themselves (*i.e.* $\rho_B = \bigotimes_\alpha \rho_{B\alpha}$); iv) The temperatures and tunnelling couplings of the baths satisfy the relation $\min_\alpha (k_B T_\alpha) \gg \max_\alpha (\hbar \gamma_\alpha)$ where $\gamma_\alpha = \frac{2\pi}{\hbar} \tau_\alpha^2 D_\alpha$ and D_α is the density of states (constant) for the bath α ; iii) Derive for the reduced density matrix of the impurity an equation of the form:

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

where $f_\alpha^+(\varepsilon) \equiv [1 + e^{\beta_\alpha(\varepsilon - \mu_\alpha)}]^{-1}$ and $f_\alpha^-(\varepsilon) = 1 - f_\alpha^+(\varepsilon)$.

2. Prove that the solution of the master equation derived in the first point can be written in the form:

$$\begin{aligned} P_0^{stat} &= \frac{1}{N} \sum_\alpha \left[\gamma_\alpha f_\alpha^-(\varepsilon_d) \right] \sum_\alpha \left[\gamma_\alpha f_\alpha^-(\varepsilon_d + U) \right] \\ P_{1\sigma}^{stat} &= \frac{1}{N} \sum_\alpha \left[\gamma_\alpha f_\alpha^+(\varepsilon_d) \right] \sum_\alpha \left[\gamma_\alpha f_\alpha^-(\varepsilon_d + U) \right] \\ P_2^{stat} &= \frac{1}{N} \sum_\alpha \left[\gamma_\alpha f_\alpha^+(\varepsilon_d) \right] \sum_\alpha \left[\gamma_\alpha f_\alpha^+(\varepsilon_d + U) \right] \end{aligned}$$

where N is the normalization factor that ensures the sum of the populations to be 1.

3. Consider now the case $U + \varepsilon_d \gg \mu_\alpha \forall \alpha$. Prove that in this case the two particle state is excluded from the stationary solution. Moreover show that the stationary reduced density matrix can be written as:

$$\rho_S^{stat} = \sum_{\alpha} \frac{\gamma_{\alpha} [f_{\alpha}^{-}(\varepsilon_d) + 2f_{\alpha}^{+}(\varepsilon_d)]}{\sum_{\alpha'} \gamma_{\alpha'} [f_{\alpha'}^{-}(\varepsilon_d) + 2f_{\alpha'}^{+}(\varepsilon_d)]} \rho_{S\alpha}^{th},$$

where $\rho_{S\alpha}^{th} = \frac{1}{Z_{\alpha}} e^{\beta_{\alpha}(H_S - \mu_{\alpha} N_S)}$ is the grandcanonical distribution of the impurity relative to the bath α .

Hint: It can be useful to consider the stationary density matrix obtained at the previous point written in the form

$$\rho_S^{stat} = \frac{1}{N} \left[|0\rangle\langle 0| + \sum_{\sigma} |1\sigma\rangle \frac{\sum_{\alpha} \gamma_{\alpha} f_{\alpha}^{+}(\varepsilon_d)}{\sum_{\alpha} \gamma_{\alpha} f_{\alpha}^{-}(\varepsilon_d)} \langle 1\sigma| \right],$$

where N is the appropriate normalization.

4. Prove analogously that, under the condition $\varepsilon_d \ll \mu_{\alpha} \forall \alpha$, the stationary reduced density matrix can be written as:

$$\rho_S^{stat} = \sum_{\alpha} \frac{\gamma_{\alpha} [2f_{\alpha}^{-}(\varepsilon_d + U) + f_{\alpha}^{+}(\varepsilon_d + U)]}{\sum_{\alpha'} \gamma_{\alpha'} [2f_{\alpha'}^{-}(\varepsilon_d + U) + f_{\alpha'}^{+}(\varepsilon_d + U)]} \rho_{S\alpha}^{th}.$$

5. Prove that with the two formulas derived at points 3 and 4 one obtains a description of the stationary state of the system $\forall \varepsilon_d$ under the only condition that $U \gg |\mu_{\alpha} - \bar{\mu}|$ and $U \gg k_B T_{\alpha}$, $\forall \alpha$ where $\bar{\mu} = \frac{1}{N_{\alpha}} \sum_{\alpha} \mu_{\alpha}$ and N_{α} is the total number of baths connected to the impurity.

2. Current through the impurity

Consider now the situation in which only 2 baths are in tunneling coupling with the impurity. If the chemical potentials of the two baths are maintained at a constant difference we obtain a net stationary current through the system.

1. Prove that the current flowing from the bath α towards the impurity is given by the formula:

$$I_{\alpha} = \gamma_{\alpha} \sum_{\sigma} \left\{ f_{\alpha}^{+}(\varepsilon_d) P_0 + [f_{\alpha}^{+}(\varepsilon_d + U) - f_{\alpha}^{-}(\varepsilon_d)] P_{1\sigma} - f_{\alpha}^{-}(\varepsilon_d + U) P_2 \right\}$$

Hint: Start with the definition of the current as the average particle variation on the impurity.

2. Prove that, according to the previous formula, the stationary currents I_{α} vanish if the two baths have the same chemical potential and the same temperature.
3. Prove that, in the stationary limit, $I_1 = -I_2$ where 1 and 2 indicate the two baths.

Frohes Schaffen!