

## Density Matrix Theory

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H33 Tuesdays, 10:15  
9.1.09 Tuesdays, 13:15

## 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  $\alpha$  we label the different baths and for simplicity we assume the same dispersion relation for the different baths. The tunnelling coupling  $\tau_{\alpha}$  is, instead, different to the different baths and we also assume a different equilibrium temperature  $T_{\alpha}$  and chemical potential  $\mu_{\alpha}$  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  $D_{\alpha}$  is the density of states (constant) for the bath  $\alpha$ ; 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  $\alpha$ .

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  $N_{\alpha}$  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  $\alpha$  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  $I_{\alpha}$  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!**