Density Matrix Theory

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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:

$$H_{\rm B} = \sum_{\alpha\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}\, c^\dagger_{\alpha\mathbf{k}\sigma} c_{\alpha\mathbf{k}\sigma},$$
$$H_{\rm T} = \sum_{\alpha\mathbf{k}\sigma} \tau_\alpha \left(c^\dagger_{\alpha\mathbf{k}\sigma} d_\sigma + d^\dagger_\sigma c_{\alpha\mathbf{k}\sigma} \right),$$

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 $H_{\rm T}$ can be treated perturbatively; ii)The impurity and the baths are uncorrelated at time $t = 0$ (*i.e.* $\rho = \rho_{\rm S} \otimes \rho_{\rm B}$). iii) The baths are not correlated between themselves (*i.e.* $\rho_{\rm B} = \bigotimes_\alpha \rho_{{\rm B}\alpha}$); iv) The temperatures and tunnelling couplings of the baths satisfy the relation $\min_\alpha(k_{\rm B}T_\alpha) \gg \max_\alpha(\hbar\gamma_\alpha)$ 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:

$$\dot{P}_0 = -\sum_\alpha \gamma_\alpha \Big\{ 2f^+_\alpha(\varepsilon_d)P_0 - \sum_\sigma f^-_\alpha(\varepsilon_d)P_{1\sigma} \Big\}$$
$$\dot{P}_{1\sigma} = -\sum_\alpha \gamma_\alpha \Big\{ [f^+_\alpha(\varepsilon_d+U) + f^-_\alpha(\varepsilon_d)]P_{1\sigma} \Big\} + \sum_\alpha \gamma_\alpha \Big\{ f^+_\alpha(\varepsilon_d)P_0 + f^-_\alpha(\varepsilon_d+U)P_2 \Big\}$$
$$\dot{P}_2 = -\sum_\alpha \gamma_\alpha \Big\{ 2f^-_\alpha(\varepsilon_d+U)P_2 - \sum_\sigma f^+_\alpha(\varepsilon_d+U)P_{1\sigma} \Big\}$$

   where $f^+_\alpha(\varepsilon) \equiv [1 + e^{\beta_\alpha(\epsilon-\mu_\alpha)}]^{-1}$ 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:

$$P_0^{stat} = \frac{1}{N}\sum_\alpha \Big[\gamma_\alpha f^-_\alpha(\varepsilon_d)\Big] \sum_\alpha \Big[\gamma_\alpha f^-_\alpha(\varepsilon_d+U)\Big]$$
$$P_{1\sigma}^{stat} = \frac{1}{N}\sum_\alpha \Big[\gamma_\alpha f^+_\alpha(\varepsilon_d)\Big] \sum_\alpha \Big[\gamma_\alpha f^-_\alpha(\varepsilon_d+U)\Big]$$
$$P_2^{stat} = \frac{1}{N}\sum_\alpha \Big[\gamma_\alpha f^+_\alpha(\varepsilon_d)\Big] \sum_\alpha \Big[\gamma_\alpha f^+(\varepsilon_d+U)\Big]$$

   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:

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

where $\rho_{\mathrm{S}\alpha}^{th} = \frac{1}{Z_\alpha} e^{\beta_\alpha (H_{\mathrm{S}} - \mu_\alpha N_{\mathrm{S}})}$ is the grancanonical 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

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

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:

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

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 $U \gg k_{\mathrm{B}} T_\alpha$, $\forall \alpha$ 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!