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 12

1. Anderson-Holstein model

The Anderson-Holstein model is the archetypal model to investigate the effect of vibrations on the transport characteristics of a nanojunction. It is a variation of the Anderson impurity model studied so far. The presence of the mechanical degree of freedom introduces a modification in the system Hamiltonian which now reads:

$$\begin{aligned} H_{\text{sys}} = &\sum_{\sigma} \epsilon_\sigma d_\sigma^\dagger d_\sigma + eV_{\text{g}}\hat{N} + \frac{U}{2}\hat{N}(\hat{N}-1) \\ &+ \hbar\omega(a^\dagger a + \tfrac{1}{2}) + g\hat{N}(a^\dagger + a) \end{aligned} \tag{1}$$

where $a^\dagger$ creates an excitation of the vibronic mode of frequency ω, while g measures the coupling between the charge on the impurity $\hat{N} = \sum_\sigma d_\sigma^\dagger d_\sigma$ and the mechanical coordinate of the vibrational mode $\propto (a^\dagger + a)$. The leads and tunnelling Hamiltonians are identical to the ones presented in the Sheet 7.

1. Find the many-body spectrum and the corresponding eigenstates of the system Hamiltonian H_{sys}. In particular, demonstrate that the latter can be labelled using the same three quantum numbers charge, spin and number of vibronic excitations as for the non interacting case (i.e. when $g = 0$). Hint: It could be useful to consider the following (canonical) transformation:

$$\tilde{H}_{\text{sys}} = \mathrm{e}^{S} H_{\text{sys}} \mathrm{e}^{-S} \tag{2}$$

   where $S = \frac{g}{\hbar\omega}\hat{N}(a^\dagger - a)$. Start by proving that $\mathrm{e}^{\pm S}$ is a unitary operator and calculate the spectrum and eigenstates of $\tilde{H}_{\text{sys}}$. What is the relation between the spectrum and the eigenstates of $\tilde{H}_{\text{sys}}$ and H_{sys} ?

2. Give a physical interpretation of the form of the eigenstates corresponding to the different particle numbers. A hint to the correct interpretation is given by the calculation of the expectation values $\langle N, S_z, m|\hat{x}|N, S_z, m\rangle$ where $N = 0, 1, 2$ is the particle number on the impurity, $S_z = 0, \uparrow, \downarrow$ is the spin on the impurity and m is the number of vibrational quanta.

3. Write the GME for the reduced density matrix in the eigenbasis of the system Hamiltonian. Assume the coupling to the leads to be so weak that you can reduce it to an equation for populations only. Write the equations in terms of the function $F(\lambda, m, m') := \langle m| \exp\left[\lambda(a^\dagger - a)\right]|m'\rangle$, where $\lambda = \frac{g}{\hbar\omega}$ and $|m\rangle$ is the m^{th} excited state of an harmonic oscillator of frequency ω.

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4. Prove that the average particle current through the lead α can be written in the form:

$$\begin{aligned} I_\alpha = & \sum_{n,\,m,\,\sigma} \Gamma_\sigma f_\alpha^+[\epsilon_\sigma + \hbar\omega(m-n-\lambda^2)]|F(\lambda,n,m)|^2 P_{0,\,n} \\ & + \sum_{n,\,m,\,\sigma} \Gamma_{\bar{\sigma}} f_\alpha^+[\epsilon_{\bar{\sigma}} + U + \hbar\omega(m-n-3\lambda^2)]|F(\lambda,n,m)|^2 P_{\sigma,\,n} \\ & - \sum_{n,\,m,\,\sigma} \Gamma_\sigma f_\alpha^-[\epsilon_\sigma + \hbar\omega(m-n-\lambda^2)]|F(\lambda,n,m)|^2 P_{\sigma,\,n} \\ & - \sum_{n,\,m,\,\sigma} \Gamma_\sigma f_\alpha^-[\epsilon_\sigma + U + \hbar\omega(m-n-3\lambda^2)]|F(\lambda,n,m)|^2 P_{2,\,n} \end{aligned} \tag{3}$$

where $P_{0/\sigma/2,\,n}$ is the probability for the system to be in the electronic state $0/\sigma/2$ and with n vibronic excitations, $f_\alpha^\pm$ is the Fermi function of the α lead and $\Gamma_\sigma = \frac{2\pi}{\hbar} D_{\alpha\sigma}|\tau|^2$ is the bare tunnelling rate from the lead α of an electron with spin σ, being $D_{\alpha\sigma}$ the corresponding density of states at the Fermi level.

5. Consider now the conductance through the nanojunction. In particuar, calculate the height and position of the two Coulomb oscillations (in correspondance to the $0 \leftrightarrow 1$ and $1 \leftrightarrow 2$ transitions) as a function of the electromechanical coupling g. The effect you will obtain is known under the name of Franck-Condon blockade and was theoretically discovered in 2005 (J. Koch and F. von Oppen, *Phys. Rev. Lett.* **94**, 206804 (2005).)

Frohes Schaffen!