University of Regensburg Winter Term 18/19

Quantum theory of condensed matter II

Mesoscopic physics (Quantum transport)

Prof. Milena Grifoni	Tue	8:00 - 10:00	9.2.01
	Fri	12:00 - 14:00	9.2.01
PD Dr. Andrea Donarini	Tue	10:00 - 12:00	5.0.21

Sheet 11

1. Self consistent solution of the Anderson impurity model

The Anderson impurity model consists of a single interacting level which can exchange electrons via tunnelling events to two reservoirs. The Hamiltonian for this system reads:

$$H = H_{\mathrm{S}} + H_{\mathrm{T}} + H_{\mathrm{res}} \tag{1}$$

where

$$\begin{aligned} H_{\mathrm{S}} &= \sum_{\sigma} \varepsilon_\sigma n_\sigma + U n_\uparrow n_\downarrow \\ H_{\mathrm{T}} &= \sum_{\alpha k \sigma} t_\alpha \, c^\dagger_{\alpha k \sigma} d_\sigma + H.c. \\ H_{\mathrm{res}} &= \sum_{\alpha k \sigma} \varepsilon_k c^\dagger_{\alpha k \sigma} c_{\alpha k \sigma} \end{aligned} \tag{2}$$

while d_σ destroys the impurity electron of spin $\sigma = \uparrow, \downarrow$, $n_\sigma = d^\dagger_\sigma d_\sigma$, and $\alpha =$ L, R labels the reservoirs. Using the equation of motion method with an appropriate truncation, you have already demonstrated in the lecture that the retarded Green's function for the impurity in presence of the reservoirs can be written as:

$$G^r_{\sigma\sigma'}(\omega) = \delta_{\sigma\sigma'} \left[\frac{1 - \langle n_{\bar\sigma} \rangle}{\omega - \varepsilon_\sigma - \Sigma^r(\omega)} + \frac{\langle n_{\bar\sigma} \rangle}{\omega - \varepsilon_\sigma - U - \Sigma^r(\omega)} \right] \tag{3}$$

where we have introduced the notation $\bar\sigma = -\sigma$ for the spin and $\Sigma^r(\omega)$ is the retarded tunnelling self-energy given by:

$$\Sigma^r(\omega) = \sum_k \frac{|t_L|^2 + |t_R|^2}{\omega - \varepsilon_k + i\eta} \tag{4}$$

The average occupation of the impurity $\langle n_\sigma \rangle$ can be calculated by solving the equation:

$$\langle n_\sigma \rangle = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} f(\omega) A_\sigma(\omega) \tag{5}$$

where the spectral function $A_\sigma(\omega)$ is defined as $A_\sigma(\omega) = -2\mathrm{Im}[G^r_{\sigma\sigma}(\omega)]$ and $f(\omega) = \frac{1}{1+\exp(\frac{\omega-\mu_0}{k_B T})}$ is the Fermi function calculated at the equilibrium chemical potential μ_0 and temperature T.

1. Assume a spin symmetric system $\varepsilon_\uparrow = \varepsilon_\downarrow = \varepsilon_d$ at temperature $T = 0$. Prove that the average occupation of the impurity reads, in this limit:

$$\langle n_\uparrow \rangle = \langle n_\downarrow \rangle = \frac{n_0}{1 + n_0 - n_U} \tag{6}$$

where $n_0 = \frac{1}{2} - \frac{1}{\pi}\mathrm{atan}(2\frac{\varepsilon_d - \mu_0}{\hbar\Gamma})$ and $n_U = \frac{1}{2} - \frac{1}{\pi}\mathrm{atan}(2\frac{\varepsilon_d + U - \mu_0}{\hbar\Gamma})$ and $\hbar\Gamma = -2\mathrm{Im}[\Sigma^r(\omega)]$ which is independent of the energy ω in the wide band limit. **(2 Points)**

2. Calculate the conductance through the Anderson impurity in the same limits considered in the previous point. You should start from the formula proved in the lecture:

$$G = e^2 \sum_\sigma \int \frac{d\xi}{2\pi} \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} A_\sigma(\xi) \left(-\frac{\partial f}{\partial \xi} \right) \tag{7}$$

where $\Gamma_\alpha = \frac{2\pi}{\hbar} |t_\alpha|^2 \mathcal{D}_\alpha$ and $\mathcal{D}_\alpha$ is the density of states of the reservoir α assumed constant in the range of relevant energies. Plot the result as a function of ε_d and Γ. Which is the role of the interaction parameter U? How are the conductance peaks depending on the parameter Γ ?
Hint: The following relation could be useful:

$$\frac{d}{dx}\theta(x) = \delta(x)$$

where $\theta(x)$ is the Heaviside function and $\delta(x)$ the Dirac distribution. **(2 Points)**

3. Consider now the spin symmetric system in the limit $\Gamma \ll k_B T$. Prove that the equation Eq.(6) is still valid, given that the following new definition of the parameters n_0 and n_U is taken: $n_0 = f(\varepsilon_d)$ and $n_U = f(\varepsilon_d + U)$. Calculate the conductance in this second parameter range and plot it as a function of ε_d and T. Which is the T dependence of the conductance peaks?

Hint: The following relation could be useful:

$$\lim_{\eta \to 0} \frac{\eta}{x^2 + \eta^2} = \pi \delta(x)$$

(2 Points)

2. Role of the interaction in the transport characteristics of SET

Consider the three papers listed below. The three of them deal with effects of interaction in the trasnport through single electron transistors (SET's). The parameters regime are, though, quite different.

Y. Meir, N. S. Wingreen, and P. A. Lee
Transport through a Strongly Interacting Electron System: Theory of Periodic Conductance Oscillations
Phys. Rev. Lett. **66** 3048 (1991)

D. Goldhaber-Gordon, H. Shtrikman, D. Mahalu, D. Abusch-Magder, U. Meirav and M. A. Kastner
Kondo effect in a single-electron transistor
Nature **391** 156 (1998)

H. W. Ch. Postma, T. Teepen, Z. Yao, M. Grifoni, C. Dekker
Carbon Nanotube Single-Electron Transistors at Room Temperature
Science **293** 76 (2001)

1. Do you recognize any of the conductance features calculated in the previous exercise?
2. Which is the fingerprint of the Kondo effect in single electron transistors? In which parameters regime (relation between U, $\hbar\Gamma$, $k_B T$) do you expect this effect to emerge?
3. Which characteristic feature of the conductance allows to conclude that the Coulomb interaction *in the leads* cannot be neglected in the carbon nanotube single electron transistor presented in the third paper?

Frohes Schaffen!