Universität Regensburg Wintersemester 13-14

Density Matrix Theory

Prof. Andrea Donarini 5.0.21, Tuesdays, 10:15

Sheet 10

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1. Single electron transistor: Transport through a metallic island

In the previous Sheet you have calculated the master equation for a metallic island in weak tunnelling coupling to metallic leads and capacitively coupled to a gate. This time you will consider the transport characteristics of such a device and calculate them numerically. The starting point are the Eq. (9) and (10) in Sheet 9:

$$\dot{P}_N = -(\Gamma_{N\to N+1} + \Gamma_{N\to N-1})P_N + \Gamma_{N+1\to N}P_{N+1} + \Gamma_{N-1\to N}P_{N-1} \tag{1}$$

where

$$\begin{aligned} \Gamma_{N\to N+1} &= \sum_{\alpha\sigma} \gamma_\alpha f(E(N+1) - E(N) - \mu_\alpha) \\ \Gamma_{N\to N-1} &= \sum_{\alpha\sigma} \gamma_\alpha f(E(N-1) - E(N) + \mu_\alpha) \end{aligned} \tag{2}$$

are the tunnelling rates and $f(E) = En_B(E)$ with n_B the Bose function $n_B(x) = (e^\beta x - 1)^{-1}$. Moreover $\gamma_\alpha = 2\pi/\hbar D_\alpha D_{\text{sys}}|\tau|^2$ and $E(N)$ is the energy of the N-particle manybody ground state of the metallic island. One can visualize this dynamical system as a chain of states with probability flowing in both directions.

1. Prove that the current through the metallic island can be written as:

$$I_\alpha = e\sum_N \left(\Gamma^\alpha_{N\to N+1} - \Gamma^\alpha_{N\to N-1}\right) P_N \tag{3}$$

   where $\Gamma^\alpha_{N\to N\pm 1}$ derives from equation (2) by omitting the sum on the lead index α.

2. Calculate the asymptotic behaviour of the function $f(E)$ introduced in Eq. (2) in the limit $E \to \pm\infty$ and calculate also the limit $E \to 0$. Compare now the energy dependance of the rates $\Gamma_{N\to N+1}$ and $\Gamma_{N+1\to N}$. Conclude that, in equilibrium ($\mu_L = \mu_R = \mu_0$) and assuming $\mu_{\text{sys}} = \mu_0$, the number of electron on the metallic island can be estimated by $N_{eq} \approx -\frac{eV_g}{U}$.

3. The stationary state for the probabilities P_N is obtained in the so called detailed balance, when the flow of probability in and out each of the states with N electrons balances out. This condition is expressed by the equation:

$$\Gamma_{N\to N+1}P_N = \Gamma_{N+1\to N}P_{N+1} \tag{4}$$

   Calculate numerically the stationary solution of Eq. (1) in the limit in which $\mu_{L,R} = \mu_{\text{sys}} \pm V_b/2$. Hint: Start considering $P_{N_{eq}} = 1$ where N_{eq} is the integer that approximates at best the equation $N = -\frac{eV_g}{U}$. Calculate the probabilities of the neighboring states by detailed balance. Repeat the operation and stop when $P_M < \epsilon$ for a given convergence parameter ϵ. Do not forget to consider both $N > N_{eq}$ and $N < N_{eq}$. Finally normalize the result such that the sum of the relevant probabilities equals 1.

4. Calculate the current as a function of the bias and gate voltage. Plot the result for different temperatures.

5. Calculate also the differential conductance and plot it as a function of bias and gate voltage. Compare the results with the stability diagram for an Anderson impurity model considered in the Sheet 8.

Frohes Schaffen!