

Density Matrix Theory

Lectures	Tue	12:00 - 13:30	PHY 5.0.20
	Thu	10:15 - 12:00	PHY 9.1.09
Exercises	Fri	10:15 - 12:00	PHY 5.0.21

Sheet 8

1. Nakajima-Zwanzig in interaction picture

Consider a system-bath described by the Hamiltonian:

$$H = H_S + H_B + H_T$$

where $[H_S, N_S] = [H_B, N_B] = 0$ being N_S and N_B respectively the system and bath number operators. Moreover, assume the tunnelling Hamiltonian H_T of the form:

$$H_T = t \sum_{ik\sigma} c_{k\sigma}^\dagger d_{i\sigma} + h.c.$$

where $c_{k\sigma}^\dagger$ creates a particle with spin σ and momentum k in the bath and $d_{i\sigma}$ destroys a particle with spin σ in the system orbital i . Prove that, if the total density matrix is factorized at the time $t = 0$ in which all representations coincide (i.e. $\rho(0) = \rho_S \otimes \rho_B$ with ρ_B the thermal equilibrium density operator) the following relation holds:

$$\mathcal{P}\dot{\rho}_I(t) = \int_0^t ds \mathcal{P}\mathcal{L}_{T,I}(t)\mathcal{G}_{Q,I}(t,s)\mathcal{L}_{T,I}(s)\mathcal{P}\rho_I(s)$$

where

$$\mathcal{G}_{Q,I}(t,s) = T_{\leftarrow} \exp \left[\int_s^t dt' \mathcal{Q}\mathcal{L}_{T,I}(t') \right],$$

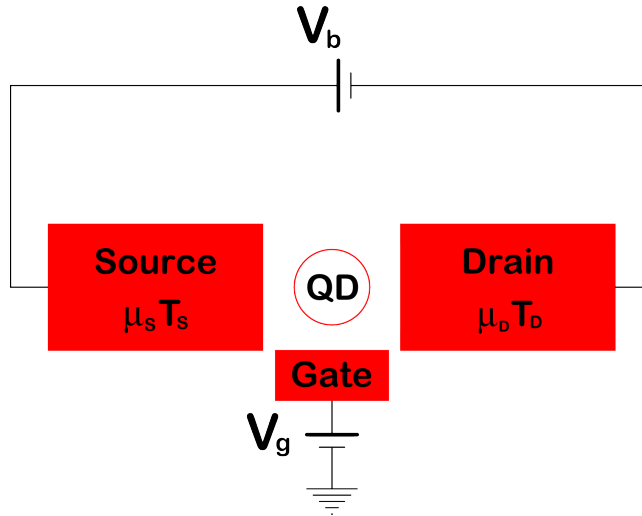
$$\mathcal{P}[\bullet] = \text{Tr}_B\{\bullet\} \otimes \rho_B, \quad \mathcal{Q} = 1 - \mathcal{P}, \quad \text{and} \quad \mathcal{L}_{T,I}(t)[\bullet] = -\frac{i}{\hbar}[H_{T,I}(t), \bullet].$$

2. Single electron transistor (SET)

Consider the device shown in the figure below. A quantum dot is coupled to three electrodes. In particular, we assume that the quantum dot can exchange electrons with the source and drain electrodes via tunnelling processes, while coupling with the gate only capacitive. It is the simplest example of single electron transistor. In first approximation one can describe the system via the two baths Anderson impurity Hamiltonian introduced in the previous sheet. The bias through the system is associated to the difference in the chemical potential of the leads by the relation $eV_b = \mu_L - \mu_R$, where e is the electron charge. The potential drop across the structure depends on the capacitive coupling between the dot and the leads. We introduce the effect of the gate via a modification of the Hamiltonian for the impurity:

$$H_S = \sum_{\sigma} (\varepsilon_d + e\alpha_g V_g) d_{\sigma}^{\dagger} d_{\sigma} + U n_{\uparrow} n_{\downarrow},$$

where e is the electron charge, V_g is the electrostatic potential of the gate electrode and α_g describes the strength of the capacitive coupling.



1. Assume that the electrostatic potential drops symmetrically at the interface between the quantum dot (QD) and the source and between the QD and the drain. Determine for which bias and gate voltages current is flowing/not flowing through the system. Plot the results as lines in a bias vs. gate voltage plane. Consider the lowest non vanishing perturbative limit in the tunnelling.

Hint: In the limit proposed by the exercise the current can flow only via sequential tunnelling events separately at the source and at the drain. Use energy conservation for each event separately to determine the requested conditions on the gate and the bias.

2. Write the master equation for the SET. Verify that the conditions derived at the previous point are the same that make the Fermi functions present in the equations turn from 0 to 1 or vice versa. Why?
3. In the Sheet 6 we have already interpreted the equilibrium of the Anderson impurity in terms of its free energy. Try to do the same also for the non equilibrium situation considered here.

Hint: Start representing the equilibrium free energy of the single electron transistor $F = H - \mu_0 N$ with $\mu_0 = \frac{\mu_S + \mu_D}{2}$ as a function of the particle number of the quantum dot. Current is flowing through the system when there is a loop of energetically allowed transitions connecting states with different particle number...

4. Typically, at low biases, the current does not flow through the SET and the number of electrons is fixed on the quantum dot. By sweeping the gate voltage one can, though change the electron number one by one. Determine the gates at which the number of electrons changes in the quantum dot and calculate the conductance for those “resonant” conditions.

Hint: Use the fact that, for a two terminal device $I_D = -I_S$ and define the current as $I = (I_S - I_D)/2$.

5. The phenomenon that you just rediscovered in the previous point is know as “Coulomb blockade”. What happens if $U = 0$? Do you think that the name is justified?
6. Write a program that calculates the stationary current across the single level quantum dot described so far as a function of bias and gate voltage. Plot the result as a three dimensional map. Make the three dimensional map also for the differential conductance

$$G(V_b, V_g) \equiv \frac{dI(V_b, V_g)}{dV_b}$$

and the populations of the different many-body states of the quantum dot. Comment the result.