Tutorials of Theoretical Condensed Matter 2019-2020

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1 Model for a quantum dot coupled to reservoirs in equilibrium

We consider a quantum dot, supposed to be small enough that we can keep only one electronic level, denoted by $|d\rangle$, on this quantum dot. We assume that this dot is coupled to two infinite electronic reservoirs R_a and R_b, on which we neglect electron-electron interactions. We also assume that each reservoir has a continuous single particle spectrum extending from $-\infty$ to ∞, and we do not take into account the electronic spin degree of freedom. The dot is coupled to both reservoirs by single electron tunneling processes. This motivates the following single-particle Hamiltonian $H_{\text{sp}} = H_0 + V$:

$$\begin{aligned} H_0 &= \epsilon_d |d\rangle\langle d| + \int_{-\infty}^{\infty} d\epsilon \epsilon (|\epsilon, a\rangle\langle \epsilon, a| + |\epsilon, b\rangle\langle \epsilon, b|) \\ V &= \int_{-\infty}^{\infty} d\epsilon \, (v_a(\epsilon)(|\epsilon, a\rangle\langle d| + |d\rangle\langle \epsilon, a|) + v_b(\epsilon)(|\epsilon, b\rangle\langle d| + |d\rangle\langle \epsilon, b|)) \end{aligned}$$

We assume that single particle states in the reservoirs are orthonormal, i.e. they are normalized according to:

$$\langle \epsilon, i|\epsilon', j\rangle = \delta_{ij}\delta(\epsilon - \epsilon'), \quad i, j \in \{a, b\}$$

To simplify expressions, we also suppose that tunneling amplitudes $v_a(\epsilon), v_b(\epsilon)$ are all real.

1. Intuitively, what do you expect for the $|d\rangle$ level, when the tunnel couplings $v_a(\epsilon), v_b(\epsilon)$ are switched on ?

2. Give the expression of the retarded Green's function $G(\omega) = (\omega - H_{\text{sp}} + i\eta)^{-1}$ as a function of $G_0(\omega)$ (the retarded Green's function for H_0) and of V.

3. Calculate explicitely $G_0(\omega)$.

4. Show that the diagonal matrix element of $G(\omega)$ has the form $\langle d|G(\omega)|d\rangle = (\omega - \epsilon_d - \Sigma(\omega) + i\eta)^{-1}$ and give the expression of the *self-energy* $\Sigma(\omega)$.

5. Introducing fermionic creation operators $d^\dagger, a^\dagger_\epsilon, b^\dagger_\epsilon$ associated to single particle states $|d\rangle, |\epsilon, a\rangle, |\epsilon, b\rangle$, and the corresponding annihilation operators $d, a_\epsilon, b_\epsilon$, write down the second-quantized version H of H_{sp}.

6. We suppose now that the system is in equilibrium at zero temperature, with all the single particle states filled up to the chemical potential μ. This forms a non-interacting Fermi sea. Let us denote by $|\text{FS}\rangle$ the corresponding many-electron state. Give a general expression for the expectation value $\langle \text{FS}|d^\dagger d|\text{FS}\rangle$ as a function of $G(\omega)$ and μ.

7. To proceed further, we assume that tunneling amplitudes $v_a(\epsilon), v_b(\epsilon)$ are independent of ϵ, and we neglect the real part of $\Sigma(\omega)$. Give then an explicit expression for $\langle \mathrm{FS}|d^\dagger d|\mathrm{FS}\rangle$ as a function of ϵ_d and draw a plot of this function. We suggest the following notations: $\Gamma_a \equiv \pi v_a^2, \Gamma_b \equiv \pi v_b^2$, $\Gamma = \Gamma_a + \Gamma_b$.

2 Out of equilibrium steady state

We wish now to study the situation when reservoirs R_a and R_b have different chemical potentials μ_a and μ_b. The first task is to generalize the notion of Fermi sea to this out of equilibrium situation. Because the spectrum is continuous, we use the same procedure as in quantum scattering theory, and obtain the scattering states $|\Psi_{\epsilon,a}\rangle$, $|\Psi_{\epsilon,b}\rangle$ as solutions of the so-called Lippmann-Schwinger equations:

$$|\Psi_{\epsilon,i}\rangle = |\epsilon, i\rangle + (\epsilon - H_0 + i\eta)^{-1} V |\Psi_{\epsilon,i}\rangle, \quad i \in \{a, b\}$$

As usual, the small positive parameter η is supposed to go to zero in the end.

In the rest of the problem, we will take for granted that these scattering states are orthonormal and complete, so:

$$\langle \Psi_{\epsilon,i}|\Psi_{\epsilon',j}\rangle = \delta_{ij}\delta(\epsilon - \epsilon')$$

$$\mathbf{I} = \int_{-\infty}^{\infty} d\epsilon \left(|\Psi_{\epsilon,a}\rangle\langle\Psi_{\epsilon,a}| + |\Psi_{\epsilon,b}\rangle\langle\Psi_{\epsilon,b}|\right)$$

8. Give explicitely the solution of these equations. We suggest the following notations:

$$\begin{aligned} |\Psi_{\epsilon,a}\rangle &= |\epsilon, a\rangle + x_a(\epsilon)|d\rangle + \int_{-\infty}^{\infty} d\epsilon' \left(y_{aa}(\epsilon', \epsilon)|\epsilon', a\rangle + y_{ba}(\epsilon', \epsilon)|\epsilon', b\rangle\right) \\ |\Psi_{\epsilon,b}\rangle &= |\epsilon, b\rangle + x_b(\epsilon)|d\rangle + \int_{-\infty}^{\infty} d\epsilon' \left(y_{ab}(\epsilon', \epsilon)|\epsilon', a\rangle + y_{bb}(\epsilon', \epsilon)|\epsilon', b\rangle\right) \end{aligned}$$

   Can you see some connection with the Green's function $G(\omega)$ of the first part ?

9. The out of equilibrium Fermi sea $|\mu_a, \mu_b\rangle$ is naturally constructed by filling all scattering states $|\Psi_{\epsilon,i}\rangle$ up to $\epsilon = \mu_i$ for $i = a, b$. We wish to implement this idea in the language of second quantization. For this, we intoduce two continuous families of fermionic creation and annihilation operators $A^\dagger(\epsilon), B^\dagger(\epsilon)$ and $A(\epsilon), B(\epsilon)$ which are associated to single particle scattering states $|\Psi_{\epsilon,a}\rangle$, $|\Psi_{\epsilon,b}\rangle$. How are these operators related to the initial ones $d^\dagger, a^\dagger(\epsilon), b^\dagger(\epsilon)$ and $d, a(\epsilon), b(\epsilon)$? What are their anticommutation relations ?

10. Express $d^\dagger$ in terms of $A^\dagger(\epsilon), B^\dagger(\epsilon)$, and d in term of $A(\epsilon), B(\epsilon)$.

11. What are the expectation values $\langle \mu_a, \mu_b|A^\dagger(\epsilon)A(\epsilon')|\mu_a, \mu_b\rangle$ and $\langle \mu_a, \mu_b|B^\dagger(\epsilon)B(\epsilon')|\mu_a, \mu_b\rangle$?

12. From this, deduce a general expression for $\langle \mu_a, \mu_b|d^\dagger d|\mu_a, \mu_b\rangle$, and give its explicit value when $\Sigma(\omega)$ is assumed to be purely imaginary and independent of ω. Give a plot of the average electron number on the dot as a function of ϵ_d. Here we assume that $\mu_a < \mu_b$ and that $\mu_b - \mu_a$ is significantly larger than Γ_a and Γ_b. What qualitative difference do you notice, in comparison to the equilibrium case ?

13. We now want to find the steady state currents I_a and I_b flowing from the reservoirs to the dot. Quantum mechanically, these are defined as expectation values of operators $\hat{I}_a$ and $\hat{I}_b$. To find these operators, we note that they have to satisfy the charge conservation equation:
$$\frac{d\langle\Psi(t)|d^\dagger d|\Psi(t)\rangle}{dt} = \langle\Psi(t)|\hat{I}_a|\Psi(t)\rangle + \langle\Psi(t)|\hat{I}_b|\Psi(t)\rangle$$
for any many-electron state $|\Psi(t)\rangle$ evolving with the Hamiltonian H. Starting from an evaluation of the left-hand side, show that this leads to explicit expressions for the current operators $\hat{I}_a$ and $\hat{I}_b$.

14. Transform these expressions for $\hat{I}_a$ and $\hat{I}_b$ using the dressed creation and annihilation operators $A^\dagger(\epsilon), B^\dagger(\epsilon)$ and $A(\epsilon), B(\epsilon)$.

15. From these, deduce the value of $I_j = \langle\mu_a, \mu_b|\hat{I}_j|\mu_a, \mu_b\rangle$ for $j = a, b$, in particular when $\Sigma(\omega)$ is assumed to be purely imaginary and independent of ω. How do these currents depend on the dot energy ϵ_d and on the chemical potentials μ_a, μ_b ?

16. Give the expressions of the Heisenberg operators $A^\dagger(\epsilon; t), B^\dagger(\epsilon; t)$ and $A(\epsilon; t), B(\epsilon; t)$.

17. Evaluate the correlation function
$$\begin{aligned} C_{\mu_a,\mu_b}(t) &= \langle\mu_a, \mu_b|d^\dagger(t)d(t)d^\dagger(0)d(0)|\mu_a, \mu_b\rangle \\ &\quad - \langle\mu_a, \mu_b|d^\dagger(t)d(t)|\mu_a, \mu_b\rangle\langle\mu_a, \mu_b|d^\dagger(0)d(0)|\mu_a, \mu_b\rangle, \end{aligned}$$
in particular when $\Sigma(\omega)$ is assumed to be purely imaginary and independent of ω. How does this correlation function depend on the dot energy ϵ_d and on the chemical potentials μ_a, μ_b ?

3 A classical stochastic model

As this section will show, and a bit counter-intuitively, in the large bias regime where $\mu_a < \epsilon_d < \mu_b$ and $\mu_b - \mu_a$ is significantly larger than Γ_a and Γ_b, the quantum mechanical correlation function $C_{\mu_a,\mu_b}(t)$ can be very well described by a purely classical stochastic model! This model is defined as follows: the dot can be either in state 0, or in state 1. Particles can tunnel from R_b into the dot with a rate γ_b and from the dot into R_a with a rate γ_a. The probabilities to find the dot in these two states evolve then according to:
$$\begin{aligned} \frac{dP(1,t)}{dt} &= -\gamma_a P(1,t) + \gamma_b P(0,t) \\ \frac{dP(0,t)}{dt} &= \gamma_a P(1,t) - \gamma_b P(0,t) \end{aligned}$$

18. Show that this stochastic model has a unique stationary probability distribution $P_{st}(n)$, and give the expectation value of the number of particles n on the dot, and of the particle currents I_a, I_b, in this steady state.

19. What is the conditional probability $\mathcal{P}(n', t|n, 0)$ to observe a charge n' on the dot at time t, knowing that its charge was n at time 0 ?

20. The charge correlation function $C_s(t)$ for this stochastic model is defined as:

$$C_s(t) = \sum_{n,n'} n'\mathcal{P}(n',t|n,0)nP_{st}(n) - \sum_{n,n'} n'P_{st}(n')nP_{st}(n)$$

    Compute $C_s(t)$.

21. Compare the results of questions 1) and 3) in this section with those of questions 5), 8) and 10) in the previous section in the large bias regime, i.e. when $\mu_a < \epsilon_d < \mu_b$ and $\mu_b - \mu_a$ is significantly larger than Γ_a and Γ_b.

22. Do you find the result surprising ? Explain why.