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Nonlinear Effects in Electron Transport Through Multiterminal Quantum Dots

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Abstract

The development of experimental methods allows scientists to manipulate the intrinsic electron property, spin. Employing spin in technological applications seems to be of invaluable importance for example, in quantum computing. Present interest in electronic transport and spin effects in multiterminal devices is motivated by their possible applications in both microelectronic and spintronic devices. As examples, we briefly mention rectification, second harmonic generation and logic functions.

In recent work, we study a single-level quantum dot (QD) weakly coupled to a number of leads in the presence of Coulomb repulsion. The leads are collinearly magnetized or remain unpolarized. The spin degeneracy of the QD can be lifted by a magnetic field not necessarily collinear with polarizations of the electrodes. We find an analytic expression for the current in the sequential tunneling regime as well as the cotunneling correction that can modify the total current significantly. The regularization procedure for the cotunneling current is shown.

When the limit of non-interacting electrons is considered, the comparison with the exact result following from the Meir-Wingreen formula is possible. In this simplified case the importance of the higher order terms in the couplings contributing to the total current can be estimated.

Interesting effects can be observed in a three-terminal device also called a Y-branch. We analyze the current through a central junction in detail when the bias is applied in push-pull fashion, with $V_l = V$ and $V_r = -V$, to the left and right branches. It can be argued that because of the system's symmetry the current in a central branch is an even function of bias voltage. The direct calculation proofs this prediction. It can be also shown that this extra lead when unpolarized allows one to distinguish between different polarization states of the left and right electrodes.

Contents

Chapter 1

Single Level Quantum Dot

1.1 Overview

The system, we have in mind, consists of a single level quantum dot coupled to a number of leads. We allow collinear spin polarization of leads, so that some of them can be polarized while others are kept unpolarized. The polarization, if any, is assumed to be complete for the sake of simplicity. To lift the spin degeneracy we apply a magnetic field to the dot, not necessarily collinear with these of the leads. We wish to study the current through one of the junctions and its dependance on the applied voltages, the position of dot's energy states, polarization of the leads and a value and orientation of the magnetic field. Except the limiting case of noninteracting electrons, the exact solution to this problem is not known, and approximative methods are widely employed. In the typical experimental setup the coupling between the dot and the lead is of order of μeV while temperature of order of meV or higher, hence it is justified to perform perturbation expansion in a small parameter $\Gamma/k_B T$.

1.2 Model Hamiltonian

The model Hamiltonian of a quantum dot connected to any number of unpolarized leads is

$$H = H_L + H_T + H_D, \tag{1.1}$$

where

$$H_L = \sum_j H_L^j = \sum_j \sum_{k\sigma} \xi_{j,k\sigma} c^\dagger_{j,k\sigma} c_{j,k\sigma} \tag{1.2}$$

describes the uncoupled leads indexed by j and $\{c^\dagger_{j,k\sigma}, c_{j,k\sigma}\}$ form an orthogonal set of creation and annihilation operators in lead j.

We consider a single level quantum dot. A degenerate spin up/spin down state with a single electron of the orbital energy ϵ_0, splits, in presence of a magnetic field, into two states with energies $E_\uparrow = \epsilon_0 - B$ and $E_\downarrow = \epsilon_0 + B$ respectively. There is a double occupancy state of energy $E_d = 2\epsilon_0 + U$, where U is the Coulomb repulsion energy. The dot is then described by the Hamiltonian

$$H_D = \sum_\sigma (\epsilon_0 - \sigma\ B) d^\dagger_\sigma d_\sigma + U n_\uparrow n_\downarrow \tag{1.3}$$

with $\sigma = \{1, -1\}$ for spin up and spin down electron respectively, $\{d^\dagger_\sigma, d_\sigma\}$ forming a set of orthogonal creation and annihilation operators for the dot and $n_\sigma = d^\dagger_\sigma d_\sigma$ being an occupation number operator. The tunneling processes between the leads and the central region are taken into account via the tunneling Hamiltonian

$$H_T = \sum_j \sum_{k\sigma} (t_{j,k\sigma} c^\dagger_{j,k\sigma} d_\sigma + \text{h.c.}), \tag{1.4}$$

where $t_{j,k\sigma}$ is a spin-dependent tunneling amplitude.

To include a complete magnetization of one of the leads, say lead j, one should limit corresponding Hilbert space to one spin direction σ_j

$$H_L^j = \sum_j \sum_k \xi_{j,k\sigma_j} c^\dagger_{j,k\sigma_j} c_{j,k\sigma_j}. \tag{1.5}$$

The dot Hamiltonian is modified accordingly. In a spin basis of the electrodes it reads

$$H_D = \sum_\sigma \epsilon_0 d^\dagger_\sigma d_\sigma + U n_\uparrow n_\downarrow - \sum_{\sigma\sigma'} \mathbf{B}\boldsymbol{\sigma}_{\sigma\sigma'} d^\dagger_\sigma d_{\sigma'}, \tag{1.6}$$

where $\boldsymbol{\sigma}$ is a vector of Pauli matrices and we assumed that a magnetic field on the quantum dot is not necessarily parallel to polarizations of the leads.

With a simple unitary rotation

$$R = \begin{pmatrix} \cos(\frac{\phi}{2}) & \sin(\frac{\phi}{2}) \\ -\sin(\frac{\phi}{2}) & \cos(\frac{\phi}{2}) \end{pmatrix} \tag{1.7}$$

we diagonalize the dot Hamiltonian which becomes

$$H_D = \sum_\sigma (\epsilon_0 - \sigma\ B)\tilde{d}^\dagger_\sigma \tilde{d}_\sigma + U\tilde{n}_\uparrow \tilde{n}_\downarrow, \tag{1.8}$$

with operators d_σ and $\tilde{d}_\sigma$ related as follows

$$d_\sigma = \sum_{\sigma'} R_{\sigma\sigma'}\tilde{d}_{\sigma'} \tag{1.9}$$

and $\tilde{n}_\sigma$ the occupation number operators in this rotated basis.

Finally, the tunneling part of the total Hamiltonian turns out to be

$$H^j_T = \sum_{k\sigma}(t_{j,k\sigma_j} R_{\sigma_j\sigma} c^\dagger_{j,k\sigma_j}\tilde{d}_\sigma + \text{h.c.}). \tag{1.10}$$

The tunneling matrix elements depend on spin, because the states in the leads are spin–dependent. Spin–flip tunneling processes could be easily incorporated in the formalism just replacing the diagonal **t** matrix by non-diagonal one. This would modify the details but not the general behavior of a current we discuss.

It is worth noting that we implicitly assumed collinear polarization of the leads. Later we will see that it might be interesting to play with electrodes' magnetization, namely polarize some of them leaving others unpolarized.

1.3 Weak tunneling regime

1.3.1 Master equations

The easiest situation we would like to study is the sequential tunneling regime, also called the weak tunneling regime. It assumes that the time between tunneling events is the largest time scale in the problem, so that there is no coherence between successive tunneling processes. If there is no voltage bias applied, the system is in a particular state, ν, described by nothing more than the Gibbs distribution function. Imagine, however, that someone turns a knob and switches the voltage on. The situation in our system becomes a highly non-equilibrium one then, and we do need to determine the new distribution functions. In order to do so, we calculate the transition rates between different states ν. Since we consider the weak tunneling limit, the Fermi's golden rule is sufficient to tackle this problem. The rate for a transition from state ν to state μ due to tunneling through junction j is

$$\Gamma^j_{\mu\nu} = \frac{2\pi}{\hbar} \sum_{f_\mu i_\nu} \left| \langle f_\mu | H^j_T | i_\nu \rangle \right|^2 W_{i_\nu} \delta(\epsilon_{f_\mu} - \epsilon_{f_\nu}), \tag{1.11}$$

where we sum up over all configurations of the internal degrees of freedom of an initial state, i_ν, that give the state ν, weighted by a thermal distribution function W_{i_ν}, and over all configurations of the final states that give a final state μ. Having found the transitions rates, we can write down master equations describing the dynamical behavior of the distribution function P_ν:

$$\frac{d}{dt} P_0 = -\sum_{j=1}^{N} \Gamma^j_{\uparrow 0} P_0 - \sum_{j=1}^{N} \Gamma^j_{\downarrow 0} P_0 + \sum_{j=1}^{N} \Gamma^j_{0\uparrow} P_\uparrow + \sum_{j=1}^{N} \Gamma^j_{0\downarrow} P_\downarrow, \tag{1.12}$$

$$\frac{d}{dt} P_\uparrow = -\sum_{j=1}^{N} \Gamma^j_{d\uparrow} P_\uparrow - \sum_{j=1}^{N} \Gamma^j_{0\uparrow} P_\uparrow + \sum_{j=1}^{N} \Gamma^j_{\uparrow d} P_d + \sum_{j=1}^{N} \Gamma^j_{\uparrow 0} P_0, \tag{1.13}$$

$$\frac{d}{dt} P_\downarrow = -\sum_{j=1}^{N} \Gamma^j_{d\downarrow} P_\downarrow - \sum_{j=1}^{N} \Gamma^j_{0\downarrow} P_\downarrow + \sum_{j=1}^{N} \Gamma^j_{\downarrow d} P_d + \sum_{j=1}^{N} \Gamma^j_{\downarrow 0} P_0, \tag{1.14}$$

$$\frac{d}{dt} P_d = -\sum_{j=1}^{N} \Gamma^j_{\uparrow d} P_d - \sum_{j=1}^{N} \Gamma^j_{\downarrow d} P_d + \sum_{j=1}^{N} \Gamma^j_{d\uparrow} P_\uparrow + \sum_{j=1}^{N} \Gamma^j_{d\downarrow} P_\downarrow, \tag{1.15}$$

where P_0, $P_\uparrow$, $P_\downarrow$, P_d are the empty, spin up, spin down and double occupation state distribution functions respectively. The terms with a minus sign give the rate at which a given state on the left-hand side decays while the plus–sign terms describe the opposite processes. The summation runs over all the leads.

It is convenient to introduce a shorthand notation for each of the above sums $\Gamma_{\mu\nu} \equiv \sum_j \Gamma^j_{\mu\nu}$, which we will use from now on.

One can solve these equations and that is not a difficult task, but what we really need, is the distribution function P_ν in the steady state. We just have to set every time derivative equal to zero and solve the resulting set of linear equations. What appears then is that these equations are not linearly independent and we are left with three equations and four unknowns. Up to now have not used the probability conservation law

$$P_0 + P_\uparrow + P_\downarrow + P_d = 1. \tag{1.16}$$

The knowledge of distribution functions allow us to find the net current flowing through, let us say, junction j

$$J_i = -\frac{e}{\hbar}\sum_\nu (\Gamma^i_{\nu+1,\nu} - \Gamma^i_{\nu-1,\nu})P_\nu. \tag{1.17}$$

This should be understood as a difference between the number of electrons incoming to the dot and deoccupating it, times the electron charge, $-e$.

Before we proceed with the most general situation, we will look at a very simple problem. Forget for a while about a magnetic field (so we deal with a degenerated state now) and set U to be so large that the double state is never occupied, $P_d = 0$. Then, Eqs. (1.12) – (1.15) reduce to

$$\frac{d}{dt}P_0 = -\Gamma_{\uparrow 0}P_0 - \Gamma_{\downarrow 0}P_0 + \Gamma_{0\uparrow}P_\uparrow + \Gamma_{0\downarrow}P_\downarrow, \tag{1.18}$$

$$\frac{d}{dt}P_\uparrow = -\Gamma_{0\uparrow}P_\uparrow + \Gamma_{\uparrow 0}P_0, \tag{1.19}$$

$$\frac{d}{dt}P_\downarrow = -\Gamma_{0\downarrow}P_\downarrow + \Gamma_{\downarrow 0}P_0. \tag{1.20}$$

Evidently, they are linearly dependent as we have already mentioned. We can choose for example Eqs. (1.19) and (1.20) together with the probability conservation law Eq. (1.16) and get

$$P_0 = \frac{\Gamma_{01}}{2\Gamma_{10} + \Gamma_{01}}, \tag{1.21}$$

$$P_\uparrow = P_\downarrow = \frac{\Gamma_{10}}{2\Gamma_{10} + \Gamma_{01}}, \tag{1.22}$$

where we introduced $\Gamma_{01} \equiv \Gamma_{0\uparrow} = \Gamma_{0\downarrow}$ and similarly $\Gamma_{10} \equiv \Gamma_{\uparrow 0} = \Gamma_{\downarrow 0}$.

All we need are couplings, $\Gamma^i_{\mu\nu}$. Their calculation is simple but awkward and has been already preformed [2]. Therefore we cite just the result

$$\Gamma^i_{10} = \Gamma^i_{\downarrow 0} = \Gamma^i_{\uparrow 0} = \Gamma^0_i n(\epsilon - \mu_i), \tag{1.23}$$

and

$$\Gamma_{01}^i = \Gamma_i^0\big(1 - n(\epsilon - \mu_i)\big), \tag{1.24}$$

where $n(\epsilon - \mu_i)$ is the Fermi distribution function whereas $\Gamma_i^0 \equiv 2\pi|t_i|^2\rho_i$ with ρ_i – the density of states for lead i. The collinear polarizations P_i of the leads might be included by using spin–dependent tunneling rates $\Gamma_{i\sigma}^0 = \frac{1}{2}\Gamma_i^0(1 + \sigma P_i)$.

The final expression for the current is then

$$J_i = -\frac{2e}{\hbar}\frac{\Gamma_i^0 \sum_{j=1}^N \Gamma_j^0\big(n(\epsilon - \mu_j) - n(\epsilon - \mu_j)\big)}{\sum_{j=1}^N \Gamma_j^0\big(1 + n(\epsilon - \mu_j)\big)}. \tag{1.25}$$

As one might expect, the current in lead i depends on the Fermi function differences between electrode i and all others, but there is also a sum over the Fermi distributions weighted by the couplings in the denominator. *Nota bene*, if we write every Γ_i^0 as $\Gamma_i^0 = \gamma\tilde{\Gamma}_i^0$ and extract a factor γ from the above fraction, we will see that the current scales with the coefficient γ.

1.3.2 Three terminal device

In 2001, electrical properties of three–terminal ballistic junctions (TBJs) were studied [3]. It was shown that for a symmetric TBJ and finite voltages $V_l = V$, $V_r = -V$ applied in a push–pull manner, to the left and right branches, the stem voltage V_s from the central branch will always be negative.

We will investigate whether this behavior is also observed in our system. The stem current according to Eq. (1.25) is given by

$$J_s = -\frac{2e}{\hbar}\frac{\Gamma_s^0\Big(\Gamma_l^0\big(n(\epsilon - \mu_s) - n(\epsilon - \mu_l)\big) + \Gamma_r^0\big(n(\epsilon - \mu_s) - n(\epsilon - \mu_r)\big)\Big)}{\Gamma^0 + \Gamma_s^0 n(\epsilon - \mu_s) + \Gamma_l^0 n(\epsilon - \mu_l) + \Gamma_r^0 n(\epsilon - \mu_r)}. \tag{1.26}$$

Following the derivation proposed by Xu [3] we expand the Fermi distribution function up to a linear term in V_s and to the quadratic terms in V

$$n(\epsilon - \mu - eV_s) = n(\epsilon - \mu) + \frac{\partial n}{\partial \epsilon}eV_s + o(V_s^2), \tag{1.27}$$

$$n(\epsilon - \mu - eV) = n(\epsilon - \mu) + \frac{\partial n}{\partial \epsilon}eV + \frac{1}{2}\frac{\partial^2 n}{\partial \epsilon^2}(eV)^2 + o(V^4), \tag{1.28}$$

$$n(\epsilon - \mu + eV) = n(\epsilon - \mu) - \frac{\partial n}{\partial \epsilon}eV + \frac{1}{2}\frac{\partial^2 n}{\partial \epsilon^2}(eV)^2 + o(V^4), \tag{1.29}$$

where a derivative is taken with respect to the energy ϵ. *We choose the Fermi level of the stem reservoir μ to be our reference level throughout the text and in all diagrams unless specified differently.* For convenience we skipped index s.

If the couplings Γ_l and Γ_r are equal, then the linear terms in V cancel one another and the stem current becomes

$$J_s \approx -\frac{2e}{\hbar}\frac{\Gamma_s^0\Gamma_l^0}{\Gamma^0}\frac{\left(2\frac{\partial n}{\partial \epsilon}eV_s - \frac{\partial^2 n}{\partial \epsilon^2}(eV)^2\right)}{1+n(\epsilon-\mu)}. \tag{1.30}$$

In the following chapters we will be mainly interested in the stem current J_s as a function of energy levels and voltages. If the dot level is well below the Fermi level, $\epsilon \ll 0$, we can replace the Fermi distributions in the denominator with 1 so that

$$J_s = \frac{e^3}{4\hbar k_B^2 T^2}\frac{\Gamma_s^0\Gamma_l^0}{\Gamma^0}\frac{\tanh\left(\frac{\epsilon}{2k_BT}\right)}{\cosh^2\left(\frac{\epsilon}{2k_BT}\right)}V^2 + o(V^4), \tag{1.31}$$

where we set $V_s = 0$. The stem current tends to zero when temperature approaches the absolute zero or becomes sufficiently large.

To find the stem voltage V_s as a function of V, we set $J_s = 0$ in Eq. (1.30) and get

$$V_s = \frac{e}{2}\frac{n''(\epsilon,T)}{n'(\epsilon,T)}V^2 + o(V^4) = \alpha(\epsilon,T)V^2 + o(V^4), \tag{1.32}$$

where

$$\alpha(\epsilon,T) = -\frac{e}{2k_BT}\tanh\left[\frac{1}{2k_BT}(\epsilon-\mu)\right]. \tag{1.33}$$

Note that the function $\alpha(\epsilon,T)$ does not depend on couplings, since we have chosen Γ_l and Γ_r to be equal. It is also apparent that a sign of the current in the central branch depends on the levels' position with respect to the reference chemical potential μ. The above result perfectly agrees with what was derived in [3]

$$\alpha(T) = e\frac{\int G_c(\epsilon)n''(\epsilon,T)d\epsilon}{\int G_c(\epsilon)n'(\epsilon,T)d\epsilon}, \tag{1.34}$$

when we set $G_c(\epsilon) = \delta(\epsilon-\epsilon_0)$. This corresponds to the situation we are studying here, namely the current through just one energy level without broadening.

The important point is that the function $\alpha(\epsilon,T)$ ensures that there should be no current for large temperatures. On the contrary, in [3] it is emphasized that Eq. (1.34) explains the room temperature properties found experimentally for the TBJ devices. What about low–temperature behavior of $\alpha(\epsilon,T)$? It goes to zero like $\alpha(\epsilon,T) \propto \frac{1}{T^2}$, so we could expect the infinite stem current at zero temperature and obviously it is nonsense. What we missed in our derivation are the higher order terms in V_s. The higher order terms in V cannot guarantee a finite value of stem voltage at zero temperature.

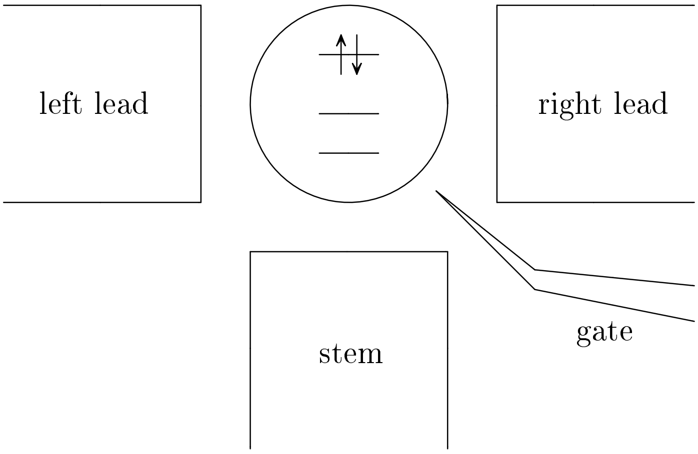

Figure 1.1: The three terminal device. The occupation number is controlled via the gate voltage V_g.

We have done the foregoing example to illustrate not only somewhat surprising behavior of the stem voltage as a function of the bias, but also to point out the problems that can arise when we cut off the Taylor series too roughly.

Now we can try to deal with a more general case of a four–level quantum dot coupled to three leads of any couplings. The solutions of Eqs. (1.12) – (1.15) are

$$P_0 = \frac{1}{D}\big(\Gamma_{0\uparrow}\Gamma_{\uparrow d}(\Gamma_{0\downarrow}+\Gamma_{d\downarrow}) + \Gamma_{0\downarrow}\Gamma_{\downarrow d}(\Gamma_{0\uparrow}+\Gamma_{d\uparrow})\big), \tag{1.35}$$

$$P_\uparrow = \frac{1}{D}\big(\Gamma_{\uparrow 0}\Gamma_{0\downarrow}(\Gamma_{\downarrow d}+\Gamma_{\uparrow d}) + \Gamma_{\uparrow d}\Gamma_{d\downarrow}(\Gamma_{\downarrow 0}+\Gamma_{\uparrow 0})\big), \tag{1.36}$$

$$P_\downarrow = \frac{1}{D}\big(\Gamma_{\downarrow 0}\Gamma_{0\uparrow}(\Gamma_{\downarrow d}+\Gamma_{\uparrow d}) + \Gamma_{\downarrow d}\Gamma_{d\uparrow}(\Gamma_{\downarrow 0}+\Gamma_{\uparrow 0})\big), \tag{1.37}$$

$$P_d = \frac{1}{D}\big(\Gamma_{d\uparrow}\Gamma_{\uparrow 0}(\Gamma_{0\downarrow}+\Gamma_{d\downarrow}) + \Gamma_{d\downarrow}\Gamma_{\downarrow 0}(\Gamma_{0\uparrow}+\Gamma_{d\uparrow})\big), \tag{1.38}$$

where

$$\begin{aligned} D = {} & (\Gamma_{\downarrow 0}\Gamma_{0\uparrow}+\Gamma_{d\uparrow}\Gamma_{\uparrow 0})(\Gamma_{\downarrow d}+\Gamma_{d\downarrow}) + (\Gamma_{0\downarrow}\Gamma_{\downarrow d}+\Gamma_{\uparrow d}\Gamma_{d\downarrow})(\Gamma_{\uparrow 0}+\Gamma_{0\uparrow}) \\ & +(\Gamma_{0\uparrow}\Gamma_{\uparrow d}+\Gamma_{\downarrow d}\Gamma_{d\uparrow})(\Gamma_{\downarrow 0}+\Gamma_{0\downarrow}) + (\Gamma_{\uparrow 0}\Gamma_{0\downarrow}+\Gamma_{d\downarrow}\Gamma_{\downarrow 0})(\Gamma_{\uparrow d}+\Gamma_{d\uparrow}) \end{aligned} \tag{1.39}$$

and

$$\Gamma^j_{\nu+1,\nu} = \Gamma^0_j n(\epsilon_{\nu+1}-\epsilon_\nu-\mu_j), \tag{1.40}$$

$$\Gamma^j_{\nu-1,\nu} = \Gamma^0_j\big(1-n(\epsilon_{\nu-1}-\epsilon_\nu-\mu_j)\big). \tag{1.41}$$

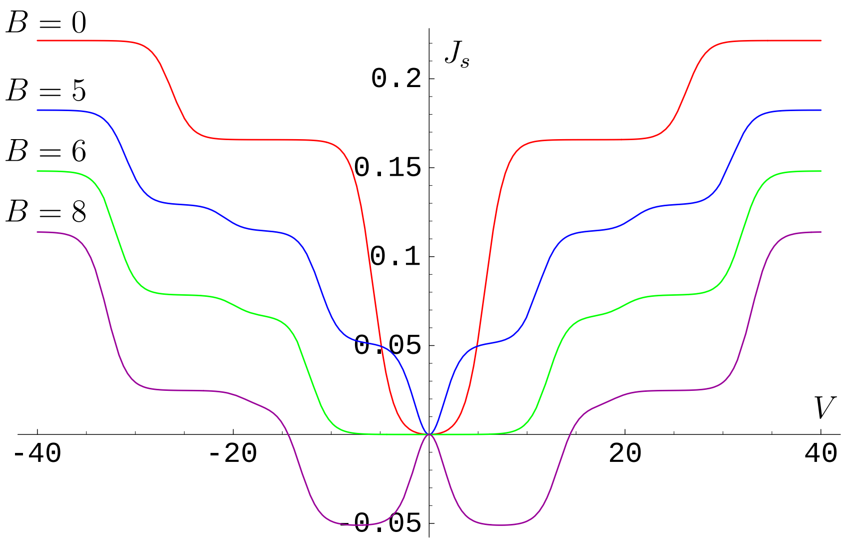

Figure 1.2: The stem current for different values of B is presented. It appears from the figure that there is a sign change in the vicinity of $V = 0$ when $B = \epsilon_0$. *See* text for explanation. Here $\epsilon_0 = 6$, $U = 20$ and $k_B T = 1$.

Using Eq. (1.25) the stem current becomes

$$J_s = -\frac{e}{\hbar}\big((\Gamma^s_{\uparrow 0} + \Gamma^s_{\downarrow 0})P_0 + (\Gamma^s_{d\uparrow} - \Gamma^s_{0\uparrow})P_\uparrow + (\Gamma^s_{d\downarrow} - \Gamma^s_{0\downarrow})P_\downarrow - (\Gamma^s_{\downarrow d} + \Gamma^s_{\uparrow d})P_d\big). \qquad (1.42)$$

The above expression is a complicated function of Fermi distributions and analytic treatment is not further possible. However, one can find very interesting results employing numerical methods.

Behavior of the stem current is highly affected by a value of the magnetic field applied to the dot — Fig. (1.2). The first appealing feature of a current–voltage characteristic is that the stem current is an even function of bias voltage. Therefore we will explain the current behavior for positive voltage. The equality, $J_s(V) = J_s(-V)$, is held until one of the following criterions is not fulfilled: the couplings Γ^0_r and Γ^0_l are different, *i.e.* due to opposite polarization of the left and right branches, or the bias is no longer applied in a push-pull fashion.

The second thing is that the current remains positive as long as $B \leq \epsilon_0$ for any bias. The character of the function changes when B crosses ϵ_0. It corresponds to a situation when a single occupancy level has the same energy as an empty state. When $B > \epsilon_0$ the hole transport dominates until the bias becomes large enough to change the current direction again – it is the apparent for $B = 8$.

The next feature are plateaus in the flow of electrons through a central brach. Consider $B = 0$ first. At zero temperature the current would be suppressed unless the $V = E_\uparrow - E_0 = E_\downarrow - E_0 = \epsilon_0$. At this point the transport through a degenerate single electron state becomes possible and we move into the Coulomb blockade regime. Excitations to the double occupation state are not possible until $V = E_d - E_\uparrow = E_d - E_\downarrow = \epsilon_0 + U$ when the next plateau is reached. Because there are no more electron states available, the current takes its final level.

In Fig. (1.2), however, the stem current is plotted for a finite temperature $k_B T = 1$ that leads to a broadening of the step-like function J_s. The above mentioned plateaus do not appear at exactly derived voltages but are smeared around these values.

For $B = 5$ the current is suppressed unless bias voltage exceeds $E_\uparrow - E_0 = \epsilon_0 - B$ and the transport through a spin up state is possible. The spin down contributes to the current from $V = E_\downarrow - E_0 = \epsilon_0 + B$. The next step appears when bias is as large as $V = E_d - E_\downarrow = \epsilon_0 + U - B$ and up-electrons are able to tunnel through the double occupied state. Eventually, the spin down electrons gain enough energy to travel through the double occupied state, $V = E_d - E_\uparrow = \epsilon_0 + U + B$.

The change in the magnetic field B affects both a vertical position of steps and their height. For fixed ϵ_0 and U there are two characteristic values of B that lead to significant modification of the $J_s(V)$ curve:

- $E_\uparrow = E_0 \Leftrightarrow B = \epsilon_0$ or $E_\downarrow = E_0 \Leftrightarrow B = -\epsilon_0$,
- $E_\uparrow = E_d \Leftrightarrow B = -(\epsilon_0 + U)$ or $E_\downarrow = E_d \Leftrightarrow B = \epsilon_0 + U$.

Only one of these two criteria in each pair can be fulfilled at the time, depending on a sign of ϵ_0 and $\epsilon_0 + U$ (as we assumed $B \geq 0$). These conditions describe for example whether the hole or the electron transport is most likely to occur for small bias. This is reflected in a sign change of the current.

Compare the case of $B = 5$ and $B = 6$. Increase of the magnetic field leads to decrease in both an initial value for which the current begins to flow and height of the first step. This happens until $E_\uparrow = E_0$ (a charge degeneracy point), or in terms of a magnetic field $B = \epsilon_0 = 6$, when the equilibrium between hole and electron transport is established and the current is suppressed. The higher bias, the more energy consuming excitations become possible and electrons begin to flow again. Here, we come up with another interesting application of the TBJ device. Tuning the magnetic field so that $B = \epsilon_0$ gives a way to measure directly electron–hole transport fluctuations. Consider the last case, $\epsilon_0 < B$ (a purple curve), when the spin up state of the dot is occupied with probability $P_\uparrow = 1$. The current is suppressed

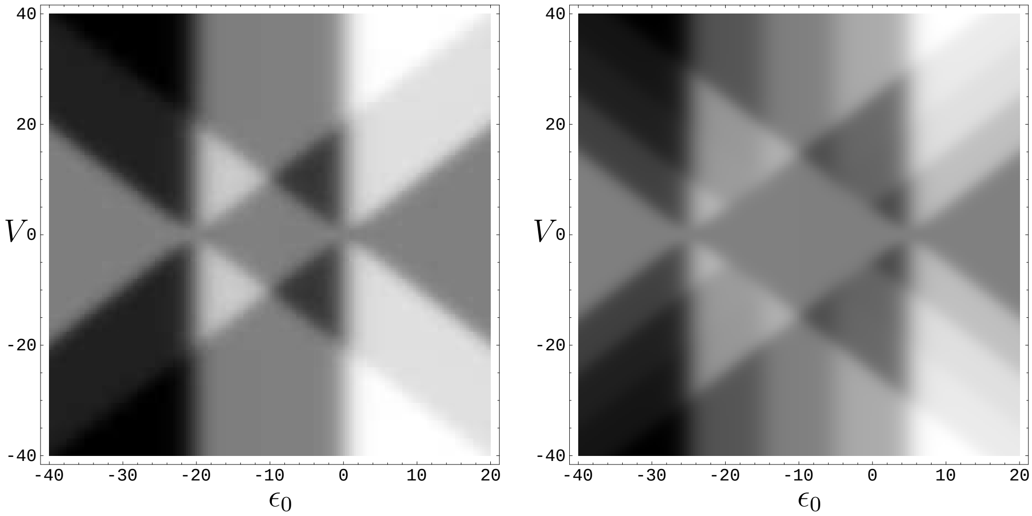

Figure 1.3: The stem current in absence of a magnetic field (on the left) and with the magnetic field $B = 5$ (on the right). All the leads are unpolarized. The interaction energy $U = 20$ and temperature $k_B T = 1$.

due to the Coulomb blockade. When the voltage reaches $V = -(\epsilon_0 - B)$ the hole transport dominates and the negative plateau appears. Again, if we considered zero temperature limit, we would experience a rapid change of a current's sign at $V = \epsilon_0 + B$, because the electron transport through spin down state would be energetically allowed and dominating. As it can be seen in Fig. (1.2), at finite temperature, this change is not so rapid and the current changes a sign somewhere between mentioned values. The next steps at $V = \epsilon_0 + U - B$ and $V = \epsilon_0 + U + B$ show up when higher transitions between dot's states are possible.

So far we have studied a cross section (along $\epsilon_0 = 6$) of what is shown in Fig. (1.3), where the stem current is plotted, in function of the electron orbital energy ϵ_0 and applied bias V. Bright regions correspond to positive values of the current while dark areas to negative ones. The stem current is an even function of bias V and an odd function of the orbital energy ϵ_0 in respect to the particle-hole symmetry line $\epsilon_0 = -U/2$.

If a magnetic field is switched off (on the left) and $\epsilon_0 < -U$ or $\epsilon_0 > 0$, the current behaves as described in text above, *i.e.* two plateaus of nonzero current are found. On the contrary, when $-U < \epsilon_0 < 0$, we expect a limited range of voltages giving nonvanishing current, $|\epsilon_0 + U| < |V| < |\epsilon_0|$ for $-U < \epsilon_0 < -U/2$, or $|\epsilon_0| < |V| < |\epsilon_0 + U|$ for $-U/2 < \epsilon_0 < 0$. If the bias voltage violates this conditions, the current flowing from the left branch to the central branch is compensated by the current from the central branch into the right one, at least as long as all the couplings are equal.

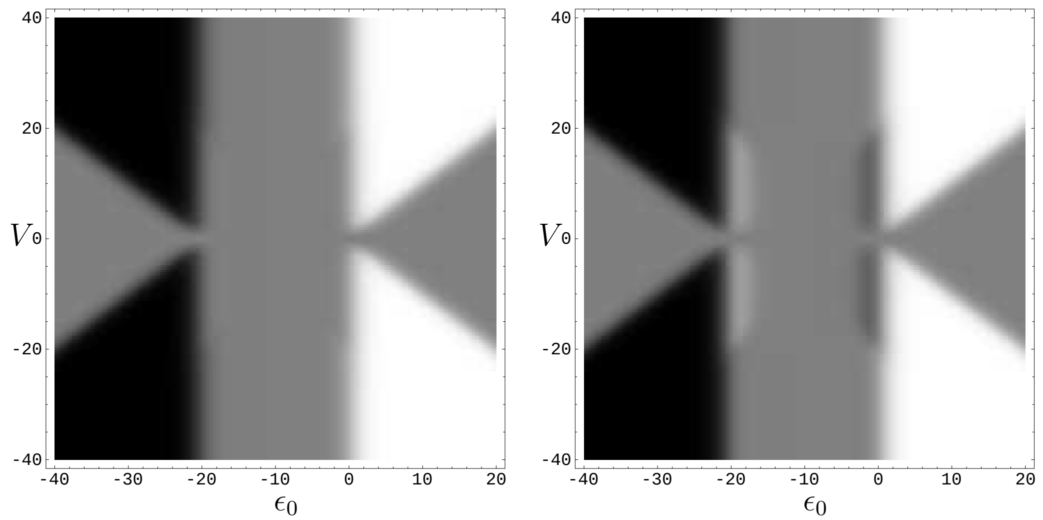

Figure 1.4: The stem current in absence of a magnetic field. The stem is unpolarized while the left and right leads are fully polarized. When the magnetic field is switched off, the relative polarization is important only (antiparallel on the left and parallel on the right). Here, $U = 20$ and $k_B T = 1$.

When the magnetic field increases, the right plot in Fig. (1.3), the area inside the diamond becomes larger and more complicated structure appears. For $\epsilon_0 > -U/2$, there are four vertical stripes distinguishable that is $-U/2 < \epsilon_0 < -U/2 + B$, $-U/2 + B < \epsilon_0 < 0$, $0 < \epsilon_0 < B$ and $\epsilon_0 > B$. The last case has been already extensively discussed while the others can be understood following the arguments in preceding text. Normally, when one considers the tunneling magnetoresistance (TMR) defined as

$$TMR \equiv \frac{J_P - J_{AP}}{J_P}, \tag{1.43}$$

where (J_{AP}) J_P is the current in (anti)parallel configuration, the two lead systems are studied. Defining the similar quantity in many leads case is rather vague. However, it seems interesting to study, for instance, the current through the central, unpolarized lead, varying magnetization of the others. If there is no magnetic field applied on the dot, the parallel and antiparallel polarizations of left and right lead are undistinguishable for overwhelming area of the stem current plotted in function of bias and gate voltage, *see* Fig. (1.4).

On the other hand, in presence of a magnetic field the picture we get is modified drastically, Fig. (1.5). The third lead gives one not only information about the relative magnetization of two remaining electrodes, but also allows one to determine polarization of each lead. This means that in this kind of

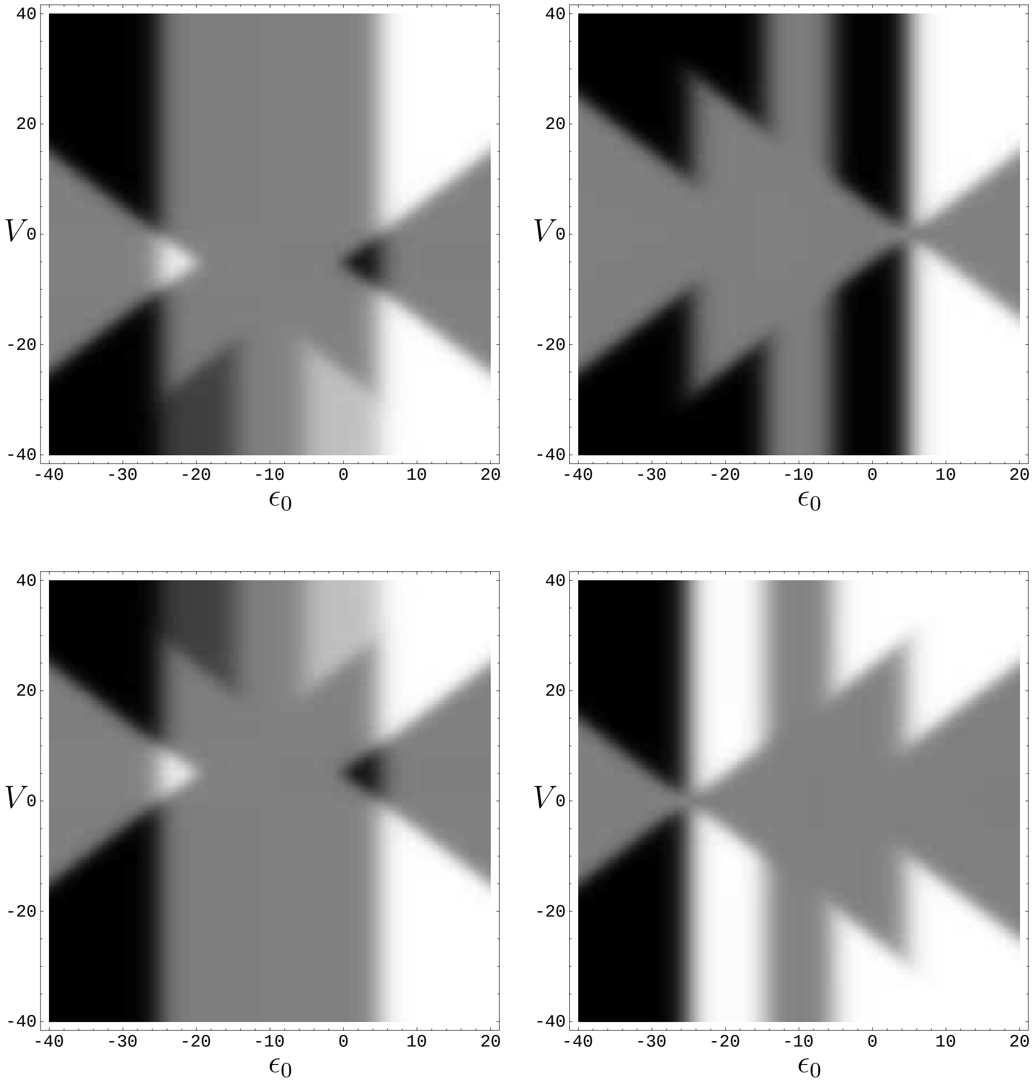

Figure 1.5: The stem current for different polarizations of leads and a magnetic field $B = 5$. Due to nonzero magnetic field, the spin symmetry is broken and the stem current is no longer an antisymmetric function of the gate voltage with respect to $\epsilon_0 = -U/2$. Here, the central branch is always unpolarized. In the left column, polarization of the left and right leads is antiparallel ($P_l = 1$, $P_r = -1$ in the upper part, and $P_l = -1$, $P_r = 1$ in lower plot). In the right column, both left and right leads are spin up polarized, $P_l = P_r = 1$ (upper picture), or spin down polarized, $P_l = P_r = -1$ (lower picture). As usual, the interaction energy $U = 20$ and temperature $k_B T = 1$.

a device we can switch among four different states and directly read out the information decoded in a two lead system with a third probe.

For antiparallel magnetization the stem current is no longer a symmetric function of bias voltage, however, the antisymmetry in gate voltage is preserved. Consider the left lead that couples to spin up states only and the right lead coupled to spin down electrons, the upper left plot in Fig. (1.5). There are several regions to be discussed. Providing $\epsilon_0 < -(U+B)$, spin up electrons move through the double occupation state if $V > -(\epsilon_0+U+B)$ into the left lead, or spin down electrons move into the right lead if $V < \epsilon_0+U-B$. In the middle region, $-(U+B) < \epsilon_0 < B$, there is no current for positive voltages, because a spin up state on the dot is always occupied by electrons coming from the stem as the energy level of this state is located below the Fermi level of the stem. Only spin down electrons can carry a charge through the dot, but they do not have enough energy to do so, because the Fermi level of the right lead is well below of this of the stem. For negative voltages the transport is also suppressed unless one of four conditions is broken:

- $\epsilon_0 + U - B < V < -(\epsilon_0 + U + B)$ and $-(U+B) < \epsilon_0 < -U$ when spin up electrons move into the stem (the white tiny triangle in the plot);
- $-(\epsilon_0 + B) < V < \epsilon_0 - B$ and $0 < \epsilon_0 < B$ when spin up electrons move from the stem (the black tiny triangle in the plot);
- $V < -(\epsilon_0 + U + B)$ and $-(U+B) < \epsilon_0 < -(U-B)$ when spin down electrons have enough energy to overcome the Coulomb blockade and move out of the central branch (the trapezoid on the left);
- $V < \epsilon_0 - U - B$ and $-B < \epsilon_0 < B$ when spin down electrons have enough energy to overcome the Coulomb blockade and move into the central branch (the trapezoid on the right);

Outside these regions, for negative voltages, the stem current is zero because either electrons do not have enough energy to move through the dot, or the currents carried in the opposite directions by spin up and spin down electrons cancel each other. Finally, for $\epsilon_0 > B$ the current flow is possible due to spin up electrons if $V > \epsilon_0 - B$, or spin down electrons if $V < -(\epsilon_0+B)$. When the magnetization of the left and right leads is switched, the whole description still holds assuming $V \to -V$ reflection, the lower left part of Fig. (1.5).

For parallel configuration the system is symmetric under left–right transformation and thus the stem current has to be a symmetric function of bias voltage. However, it is not an antisymmetric function of electron orbital energy, because the lateral branches do not couple to spin up and spin down electrons equally. If $\epsilon_0 < -(U+B)$, the spin down state is always occupied due to a spin down electron coming from the central branch. The transport is possible through the double occupation state for $V < -\epsilon_0 - U + B$. There are two regions, $-(U+B) < \epsilon_0 < -(U-B)$ and $-B < \epsilon_0 < B$, where electrons escape from the stem to one of the side branches provided $V > -\epsilon_0 + B$. In the middle stripe, $-(U-B) < \epsilon_0 < -B$, the electrons moving out of one branch and into another compensate each other and there is no net current. Eventually, there is a region of positive current, $\epsilon_0 > B$, due to electrons travelling through single occupied state into the stem. This is possible when $V > \epsilon_0 - B$. This explains the stem current characteristic for the parallel configuration when both lateral leads are spin up polarized, the upper-right plot in Fig. (1.5). The situation for switched, spin down polarization can be described by analogy, performing electron–hole transformation.

1.4 Cotunneling regime

In the cotunneling regime two electron processes come into play. An electron is transferred between lead j and lead i in two successive tunneling events, through a quantum dot. Time Δt the electron spends on the dot can be estimated from the Heisenberg uncertainty principle $\Delta t \propto \hbar/\Delta E$, where ΔE is the energy difference between the initial and intermediate state, and is much shorter than time the electron needs to tunnel sequentially. We distinguish four regimes according to the occupation of the dot. The dot might be empty, occupied by a spin up electron, a spin down electron or double occupied, depending on the location of dot's energy levels with respect to the Fermi levels of the leads. The probabilities that a given state is occupied are given by Eqs. (1.35) – (1.38).

There are two types of processes that should be considered, *i.e.* non-spin-flip processes that do not change dot's magnetization and spin-flip processes leading to reversal of spin direction. The latter contribute directly to the current as well as modify the probabilities P_σ via spin-flips caused by the interaction of the dot with a lead. We find the rates for these processes employing generalized Fermi's Golden Rule [2]

$$\Gamma_{fi} = \frac{2\pi}{\hbar}\left|\langle f|T|i\rangle\right|^2 \delta(E_f - E_i) \tag{1.44}$$

for the transition from the initial state $|i\rangle$ of energy E_i to the final state $|i\rangle$ of energy E_f. The transition operator T is defined as

$$T = H_T + H_T \frac{1}{E_i - H_0} T \tag{1.45}$$

with $H_0 = H_L + H_D$. It turns out that the first nonvanishing transition rate for the process which exchanges an electron between electrodes appears in the second order perturbation expansion. This is completely understandable since the transition operator has to be quadratic in the tunneling Hamiltonian so that two tunneling events take place. In other words the cotunneling process is quadratic in couplings, Γ.

Even if the number of leads remains unspecified, the cotunneling events occur only between pairs of the leads (as the processes taking into account nearly simultaneous exchange of electrons among more than two leads are of the higher order in Γ than Γ^2). Hence, it becomes elucidated that the cotunneling current through junction i can be expressed as the sum of the *paired currents* $J_{ij}^{(\nu)}$, *i.e.* the currents between lead i and j in regime ν, weighted by the appropriate probability P_ν

$$J_i = \sum_j \Big(\sum_\nu P_\nu J_{ij}^{(\nu)} + \sum_\sigma J_{ij}^{(\sigma),sf} \Big). \tag{1.46}$$

The summation runs over the dot's states $\nu = 0, \uparrow, \downarrow, 2$. For emphasis we divided the paired current into a non-spin-flip part $J_{ij}^{(\nu)}$ and a spin-flip part $J_{ij}^{(\sigma),sf}$, present for the single occupation only.

1.4.1 Unpolarized leads

To get a feeling of what happens in the system, we begin with the simplest case of unpolarized leads and study the case of an empty dot. The initial state $|i\rangle = |\nu_1, \ldots, \nu_N, 0\rangle$ consists of a tensor product of lead states $|\nu_i\rangle$ and the dot state $|0\rangle$. An electron can be transferred from lead i into lead j via either a spin up state or a spin down state of the dot, depending on spin of the electron entering the intermediate region. Because the final states of the leads are different $|f\rangle = |\nu_1, \ldots, \nu_i - \sigma, \ldots, \nu_j + \sigma, \ldots, \nu_N, 0\rangle = c_{i,k\sigma} c^\dagger_{j,k'\sigma}|i\rangle$, there is no interference between electron's paths and we find the rates $\Gamma^{(0)}_{j\sigma i\sigma}$ for these two processes separately and add them up to get the total tunneling rate in this regime, summing over σ. Thus, the paired current is given by

$$J_{ij}^{(0)} = -e \sum_\sigma (\Gamma^{(0)}_{j\sigma i\sigma} - \Gamma^{(0)}_{i\sigma j\sigma}) \tag{1.47}$$

that is the rate for process bringing electron from lead i to lead j, minus the rate for the opposite process, multiplied by the electron charge, $-e$. As stated in the preceding section the tunneling rate follows from the Fermi's Golden Rule. We substitute the tunneling Hamiltonian H_T into $\langle f|T|i\rangle$ and arrive at

$$\begin{aligned} I_0 \equiv \langle f|T|i\rangle &= \sum_{k_1 k_2} \langle f| t^*_{i,k_1\sigma} d^\dagger_\sigma c_{i,k_1\sigma} \frac{1}{E_i - H_0} t_{j,k_2\sigma} c^\dagger_{j,k_2\sigma} d_\sigma |i\rangle \\ &= \sum_{k_1 k_2} t^*_{i,k_1\sigma_i} t_{j,k_2\sigma_j} \frac{1}{\xi_{k\sigma} - \epsilon_\sigma} \langle \nu_i | c_{i,k\sigma} c^\dagger_{i,k_1\sigma} |\nu_i\rangle \langle \nu_j | c^\dagger_{j,k'\sigma} c_{j,k_2\sigma} |\nu_j\rangle, \end{aligned} \tag{1.48}$$

where we used decomposition of the initial state $|i\rangle = |\nu_1, \ldots, \nu_N, 0\rangle = |\nu_1\rangle|\nu_2\rangle \ldots |\nu_N\rangle|0\rangle$, leaving explicitly relevant terms with $|\nu_i\rangle$ and $|\nu_j\rangle$. According to the orthogonality relations for the lead basis, only terms with $k_1 = k$ and $k_2 = k'$ preserve the summation.

To find the tunneling rate we sum over the momentum states k (k') of the electron leaving lead i (entering lead j) and over all states of the leads, ν_i and ν_j

$$\Gamma^{(0)}_{j\sigma i\sigma} = \frac{2\pi}{\hbar} \sum_{kk'} \sum_{\nu_i \nu_j} W_{\nu_i} W_{\nu_j} |I_0|^2 \delta(\xi_{k\sigma} - \xi_{k'\sigma}), \tag{1.49}$$

where W_{ν_i} denotes the probability that lead i is in a state ν_i and $E_f - E_i = \xi_{j,k'\sigma} - \xi_{i,k\sigma}$ enters Dirac's delta.

It is noteworthy that since we deal with fermionic operators, $\langle \nu_i | c^\dagger_{i,k\sigma} c_{i,k\sigma} | \nu_i \rangle$ equals either 0 or 1 and, hence, $\left| \langle \nu_i | c^\dagger_{i,k\sigma} c_{i,k\sigma} | \nu_i \rangle \right|^2 = \langle \nu_i | c^\dagger_{i,k\sigma} c_{i,k\sigma} | \nu_i \rangle$. Skipping these squares we get

$$\begin{aligned}\Gamma^{(0)}_{j\sigma i\sigma} = \frac{2\pi}{\hbar} \sum_{kk'} |t_{i,k\sigma}|^2 |t_{j,k'\sigma}|^2 \frac{1}{(\xi_{k\sigma} - \epsilon_\sigma)^2} \delta(\xi_{k\sigma} - \xi_{k'\sigma}) \\ \times \sum_{\nu_i} \langle \nu_i | c^\dagger_{i,k\sigma} c_{i,k\sigma} | \nu_i \rangle \sum_{\nu_j} \langle \nu_j | (1 - c^\dagger_{j,k'\sigma} c_{j,k'\sigma}) | \nu_j \rangle. \end{aligned} \tag{1.50}$$

Because leads are noninteracting, W_{ν_i} satisfies

$$\sum_{\nu_i} W_{\nu_i} \langle \nu_i | c^\dagger_{i,k\sigma} c_{i,k\sigma} | \nu_i \rangle = n(\epsilon_{i,k\sigma} - \mu_i) \tag{1.51}$$

and we end up with Fermi functions. Assuming continues energy spectrum in the leads, the sum can be replaced by the integral

$$2\pi \sum_k |t_{i,k\sigma}|^2 \approx 2\pi \int_{-\infty}^{\infty} d\xi \rho_i |t_{i,\sigma}|^2 \approx \Gamma^0_{i\sigma} \int_{-\infty}^{\infty} d\xi \tag{1.52}$$

with energy independent $\Gamma_{i\sigma} \equiv 2\pi\rho_i |t_{i,\sigma}|^2$. Finally, the rate for the process bringing an electron with spin σ from lead i into lead j is

$$\Gamma^{(0)}_{j\sigma i\sigma} = \frac{1}{h} \Gamma^0_{i\sigma} \Gamma^0_{j\sigma} \int_{-\infty}^{\infty} d\xi \frac{1}{(\xi - \epsilon_\sigma)^2} n(\xi - \mu_i) \big(1 - n(\xi - \mu_j)\big). \tag{1.53}$$

and employing Eq. (1.54), the paired current through an empty dot becomes

$$J^{(0)}_{ij} = -\frac{e}{h} \Gamma^0_i \Gamma^0_j \int_{-\infty}^{\infty} d\epsilon \left(\frac{1}{(\epsilon - \epsilon_\uparrow)^2} + \frac{1}{(\epsilon - \epsilon_\downarrow)^2} \right) \big(n(\epsilon - \mu_i) - n(\epsilon - \mu_j) \big), \tag{1.54}$$

where we assumed $\Gamma^0_i = \Gamma^0_{i\uparrow} = \Gamma^0_{i\downarrow}$. The paired current through a single occupied dot may be found by analogy

$$J^{(\sigma)}_{ij} = -\frac{e}{h} \Gamma^0_i \Gamma^0_j \int_{-\infty}^{\infty} d\epsilon \left(\frac{1}{(\epsilon - \epsilon_\sigma)^2} + \frac{1}{(\epsilon - \epsilon_{\bar\sigma} - U)^2} \right) \big(n(\epsilon - \mu_i) - n(\epsilon - \mu_j) \big) \tag{1.55}$$

if one neglects inelastic processes. The expression for the paired current in presence of spin-flipping will be derived below as it needs more attention.

Eventually, the paired current in the remaining regime of double occupation reads

$$J_{ij}^{(2)} = -\frac{e}{h}\Gamma_i^0\Gamma_j^0 \int_{-\infty}^{\infty} d\epsilon \left(\frac{1}{(\epsilon-\epsilon_\uparrow - U)^2} + \frac{1}{(\epsilon-\epsilon_\downarrow - U)^2} \right) \big(n(\epsilon-\mu_i) - n(\epsilon-\mu_j) \big). \tag{1.56}$$

As long as we consider the limit of noninteracting electrons, $U = 0$, the inelastic processes do not affect the current at all, and the above description is completely sufficient. In Sec. 1.5 we will compare the perturbative result we got here with the strict result coming from two different formulations, namely Landauer-Büttiker formula and Meir-Wingreen formalism. It will be shown that for noninteracting electrons the second order perturbation theory gives an excellent estimate of this strict expression.

At the moment, however, we will calculate the cotunneling rate for the process that results in change of dot's magnetization. As mentioned before, this is possible only for single occupied state. Consider then the initial state $|i\rangle = |\nu_1, \ldots, \nu_N, \sigma\rangle$ with electron on the dot being in a state σ, and the final state$|f\rangle = |\nu_1, \ldots, \nu_i - \sigma, \ldots, \nu_j + \bar{\sigma}, \ldots, \nu_N, \bar{\sigma}\rangle = d_{\bar{\sigma}}^\dagger c_{i,k\bar{\sigma}} c_{j,k'\sigma}^\dagger d_\sigma |i\rangle$. Energy of the initial state is $E_i = E_L + \epsilon_\sigma$ while of the final state $E_f = E_L - \xi_{i,k\bar{\sigma}} + \xi_{j,k'\sigma} + \epsilon_{\bar{\sigma}}$, with E_L being an eigenvalue of the leads' Hamiltonian H_L. The transition between these states happens via two, indistinguishable channels. The amplitude I_0 for the first channel transition is

$$\begin{aligned} I_0 &\equiv \sum_{k_1 k_2} \langle f | t_{i,k_1\bar{\sigma}}^* d_{\bar{\sigma}}^\dagger c_{i,k_1\bar{\sigma}} \frac{1}{E_i - H_0} t_{j,k_2\sigma} c_{j,k_2\sigma}^\dagger d_\sigma | i \rangle \\ &= \sum_{k_1 k_2} t_{i,k_1\bar{\sigma}}^* t_{j,k_2\sigma} \frac{1}{\epsilon_\sigma - \xi_{k_2\sigma}} \langle \nu_i | c_{i,k\bar{\sigma}}^\dagger c_{i,k_1\bar{\sigma}} | \nu_i \rangle \langle \nu_j | c_{j,k'\sigma}^\dagger c_{j,k_2\sigma} | \nu_j \rangle \end{aligned} \tag{1.57}$$

and describes the processes when an electron leaves the dot, a short leaving empty state is created, and, afterwards, the next electron with the opposite spin jumps onto the dot.

The next possibility is that the second electron enters the dot, resulting in double occupation, and then the first electron jumps out, leaving the dot with a flipped spin state. This type of process is given by the amplitude I_2

$$\begin{aligned} I_2 &\equiv \sum_{k_1 k_2} \langle f | t_{j,k_2\sigma} c_{j,k_2\sigma}^\dagger d_\sigma \frac{1}{E_i - H_0} t_{i,k_1\bar{\sigma}}^* d_{\bar{\sigma}}^\dagger c_{i,k_1\bar{\sigma}} | i \rangle \\ &= \sum_{k_1 k_2} t_{i,k_1\bar{\sigma}}^* t_{j,k_2\sigma} \frac{1}{\xi_{k_1\bar{\sigma}} - \epsilon_{\bar{\sigma}} - U} \langle \nu_i | c_{i,k\bar{\sigma}}^\dagger c_{i,k_1\bar{\sigma}} | \nu_i \rangle \langle \nu_j | c_{j,k'\sigma}^\dagger c_{j,k_2\sigma} | \nu_j \rangle. \end{aligned} \tag{1.58}$$

Since, as already pointed out, it is impossible to distinguish between these two tunneling paths, we add the amplitudes and square the sum

$$\Gamma_{j\bar{\sigma}i\sigma} = \frac{2\pi}{\hbar}\sum_{kk'}\sum_{\nu_i\nu_j} W_{\nu_i}W_{\nu_j}|I_0 + I_2|^2\delta(\xi_{k'\sigma} - \xi_{k\bar{\sigma}} + \Delta_{\bar{\sigma}\sigma}), \tag{1.59}$$

where $\Delta_{\bar{\sigma}\sigma} \equiv \epsilon_{\bar{\sigma}} - \epsilon_\sigma$ is the change of the dot's energy due to the spin-flip process. Note that $\Delta_{\bar{\sigma}\sigma}$ is nonzero only in presence of an external magnetic field.

Having in mind the tips we gave in the previous calculation, the derivation of the above transition rate is now straightforward and we give just the final result

$$\Gamma_{j\bar{\sigma}i\sigma} = \frac{1}{h}\Gamma^0_{i\sigma}\Gamma^0_{j\bar{\sigma}}\int_{-\infty}^{\infty} d\xi \left(\frac{1}{\xi - \epsilon_{\bar{\sigma}} - U} - \frac{1}{\xi - \epsilon_{\bar{\sigma}}}\right)^2 \times n(\xi - \mu_i)\big(1 - n(\xi - \mu_j - \Delta_{\bar{\sigma}\sigma})\big) \tag{1.60}$$

in agreement with [4]. The important remark should be done at this point. For noninteracting electrons we expect the destructive interference so that inelastic cotunneling does not play any role and the Eqs. (1.54) – (1.56) along with Eq. (1.46) gives the whole picture. If $U > 0$, the paired current is

$$J_{ij}^{(\sigma),sf} = -e(\Gamma_{j\bar{\sigma}i\sigma} - \Gamma_{i\bar{\sigma}j\sigma}) \tag{1.61}$$

and for symmetrical couplings to spin up and spin down states, $= \Gamma_i^0 = \Gamma_{i\uparrow}^0 = \Gamma_{i\downarrow}^0$ it can be written as

$$J_{ij}^{(\sigma),sf} = -\frac{e}{h}\Gamma_i^0\Gamma_j^0\int_{-\infty}^{\infty} d\xi\left(\frac{1}{\xi - \epsilon_{\bar{\sigma}} - U} - \frac{1}{\xi - \epsilon_{\bar{\sigma}}}\right)^2\big(n(\xi - \mu_i) - n(\xi - \mu_j) + n(\xi - \mu_j)n(\xi - \mu_i - \Delta_{\bar{\sigma}\sigma}) - n(\xi - \mu_i)n(\xi - \mu_j - \Delta_{\bar{\sigma}\sigma})\big). \tag{1.62}$$

The terms containing products of the Fermi functions cancel approximately one another if $|\Delta_{\bar{\sigma}\sigma}|/k_BT \ll 1$, that is a magnetic field is small compared to temperature, which is usually a good assumption, or the bias voltage applied between lead i and lead j is small compared to the single level splitting, $|(\mu_i - \mu_j)/\Delta_{\bar{\sigma}\sigma}| \ll 1$.

To this point, we have derived all the expressions necessary to find the current in the cotunneling regime. The problem with these results is that each denominator blows up whenever energy of an electron in leads reaches excitation energy, *i.e.* energy sufficient to change occupation of the dot. Surely this divergence cannot be accepted from the physical point of view. One should realize that the energy levels always have some broadening resulting from the contact either with the surrounding (for instance through phonons) or with the leads. Before we propose a regularization method, or maybe, more precisely, the renormalization procedure later, we consider the linear response regime and make use of the fact that $|\epsilon| \ll |\epsilon_\sigma|, |\epsilon_\sigma + U|$ obtaining

$$J_{ij}^{(0)} = -\frac{e}{h}\Gamma_i^0\Gamma_j^0\left(\frac{1}{\epsilon_\uparrow^2} + \frac{1}{\epsilon_\downarrow^2}\right)\mu_{ij}, \tag{1.63}$$

$$J_{ij}^{(\sigma)} = -\frac{e}{h}\Gamma_i^0\Gamma_j^0\left(\frac{1}{\epsilon_\sigma^2} + \frac{1}{(\epsilon_{\bar{\sigma}} + U)^2}\right)\mu_{ij}, \tag{1.64}$$

$$J_{ij}^{(2)} = -\frac{e}{h}\Gamma_i^0\Gamma_j^0\left(\frac{1}{(\epsilon_\sigma + U)^2} + \frac{1}{(\epsilon_{\bar{\sigma}} + U)^2}\right)\mu_{ij} \tag{1.65}$$

for non-spin-flip cotunneling currents. Since we assumed small voltages, the terms quadratic in Fermi functions in Eq. (1.62) are omitted, and the linear response result for the inelastic scattering reads

$$J_{ij}^{(\sigma),lin} = -\frac{e}{h}\Gamma_i^0\Gamma_j^0\left(\frac{1}{\epsilon_{\bar{\sigma}}} - \frac{1}{\epsilon_{\bar{\sigma}} + U}\right)^2\mu_{ij}, \tag{1.66}$$

where $\mu_{ij} = \mu_i - \mu_j = e(V_i - V_j)$. Unfortunately, these simple results will not be sufficient if we are interested in non-linear effects appear beyond the approximation applied.

1.4.2 Regularization procedure

If one wants to proceed beyond the zero temperature limit, they need to use a more sophisticated method to cut off the infinite behavior properly. At first, consider the divergence appearing in the non-spin-flip cotunneling current. In general, the problematic integral has a form

$$\int d\xi \frac{f(\xi)}{(\xi - \xi_0)^2 + \eta^2} \equiv \int_{-\infty}^{\infty} d\xi \frac{1}{|\xi - \xi_0 + i\eta|^2}\big(n(\xi - \mu_i) - n(\xi - \mu_j)\big) \tag{1.67}$$

where, following the derivation of Turek and Matveev [5], we add an infinitesimal imaginary part, $i\eta$, to the denominator, with $\eta > 0$, and defined $f(\xi) \equiv n(\xi - \mu_i) - n(\xi - \mu_j)$. Now, the trick is to partition each of this integral into the part, that *a posteriori* will be identified with the sequential tunneling contribution, and the expression describing pure cotunneling processes

$$\begin{aligned}\int d\xi \frac{f(\xi)}{(\xi - \xi_0)^2 + \eta^2} &= \int d\xi \frac{f(\xi_0)}{(\xi - \xi_0)^2 + \eta^2} + \int d\xi \frac{f(\xi) - f(\xi_0)}{(\xi - \xi_0)^2 + \eta^2} \\ &= \frac{\pi}{|\eta|} f(\xi_0) + \lim_{\eta \to 0^+} \int d\xi \frac{f(\xi) - f(\xi_0)}{(\xi - \xi_0)^2 + \eta^2}.\end{aligned} \tag{1.68}$$

The first component of the above sum is the isolated divergence while the second one is a nicely behaving integral, which might be evaluated analytically. As the procedure leading to the final expression is quite lengthy, we refer the interested reader to App. A, and cite the result only

$$\int_{-\infty}^{\infty} \frac{d\xi}{(\xi-\xi_0)^2}\big(n(\xi-\mu_i)-n(\xi-\mu_j)\big)$$
$$\longrightarrow \Re\Big[\frac{\beta}{2\pi i}\Big(\Psi_1\Big(\frac{1}{2}-\frac{\beta}{2\pi i}(\xi_0-\mu_i)\Big)-\Psi_1\Big(\frac{1}{2}-\frac{\beta}{2\pi i}(\xi_0-\mu_j)\Big)\Big)\Big], \quad (1.69)$$

where $\Psi_n(z)$ is the polygamma function. The arrow should remind the reader that these expressions are not equal. The integral is divergent while the formula on the right of the arrow is regularized. For the sake of simplicity we introduce a shorthand notation

$$\Psi_n(\xi,\mu) \equiv \Psi_n\Big(\frac{1}{2}-\frac{\beta}{2\pi i}(\xi-\mu)\Big) \quad (1.70)$$

and list below the paired currents after regularization

$$J_{ij}^{(0)} = -\frac{e}{h}\Gamma_i^0\Gamma_j^0\Re\big[\frac{\beta}{2\pi i}\big(\Psi_1(\epsilon_\uparrow,\mu_i)-\Psi_1(\epsilon_\uparrow,\mu_j)\big)$$
$$+\frac{\beta}{2\pi i}\big(\Psi_1(\epsilon_\downarrow,\mu_i)-\Psi_1(\epsilon_\downarrow,\mu_j)\big)\big], \quad (1.71)$$

$$J_{ij}^{(\sigma)} = -\frac{e}{h}\Gamma_i^0\Gamma_j^0\Re\big[\frac{\beta}{2\pi i}\big(\Psi_1(\epsilon_\sigma,\mu_i)-\Psi_1(\epsilon_\sigma,\mu_j)\big)$$
$$+\frac{\beta}{2\pi i}\big(\Psi_1(\epsilon_{\bar\sigma}+U,\mu_i)-\Psi_1(\epsilon_{\bar\sigma}+U,\mu_j)\big)\big], \quad (1.72)$$

$$J_{ij}^{(2)} = -\frac{e}{h}\Gamma_i^0\Gamma_j^0\Re\big[\frac{\beta}{2\pi i}\big(\Psi_1(\epsilon_\uparrow+U,\mu_i)-\Psi_1(\epsilon_\uparrow+U,\mu_j)\big)$$
$$+\frac{\beta}{2\pi i}\big(\Psi_1(\epsilon_\downarrow+U,\mu_i)-\Psi_1(\epsilon_\downarrow+U,\mu_j)\big)\big]. \quad (1.73)$$

The paired current in presence of inelastic scattering, Eq. (1.62), causes much more troubles. First of all, the analytic formula can be found only for the part which is linear in Fermi functions. The quadratic terms can be neglected if relevant conditions are fulfilled, or, otherwise, a new kind of treatment is necessary. Second, the interference term appears, with $1/\xi$ divergence

$$\Big(\frac{1}{\xi-\xi_1}-\frac{1}{\xi-\xi_2}\Big)^2 = \frac{1}{(\xi-\xi_1)^2}+\frac{1}{(\xi-\xi_2)^2}-\frac{2}{\xi_1-\xi_2}\Big(\frac{1}{\xi-\xi_1}-\frac{1}{\xi-\xi_2}\Big). \quad (1.74)$$

We will show that the proposed regularization procedure works for this divergence as well. Let us focus on the linear part of Eq. (1.62)

$$J_{ij}^{(\sigma),lin} = -\frac{e}{h}\Gamma_i^0\Gamma_j^0 \int_{-\infty}^{\infty} d\xi \left| \frac{1}{\xi - \xi_1 + i\eta} - \frac{1}{\xi - \xi_2 + i\eta} \right|^2 \big(n(\xi - \mu_i) - n(\xi - \mu_j)\big). \tag{1.75}$$

The bracket was replaced here with the absolute value (coming from the Fermi's Golden Rule) and a small imaginary part $i\eta$ was put in to denominators. Expanding the expression in the modulus we obtain

$$\begin{aligned} J_{ij} = &-\frac{e}{h}\Gamma_i^0\Gamma_j^0 \int_{-\infty}^{\infty} d\xi \Bigg(\frac{1}{(\xi-\xi_1)^2+\eta^2} + \frac{1}{(\xi-\xi_2)^2+\eta^2} \\ &- 2\frac{\xi^2 - (\xi_1+\xi_2)\xi + \xi_1\xi_2 + \eta^2}{\big((\xi-\xi_1)^2+\eta^2\big)\big((\xi-\xi_2)^2+\eta^2\big)} \Bigg) \big(n(\xi-\mu_i) - n(\xi-\mu_j)\big) \end{aligned} \tag{1.76}$$

with the cross term having nice finite behavior what can be checked by a direct integration

$$\int_{-\infty}^{\infty} d\xi \frac{\xi^2 - (\xi_1+\xi_2)\xi + \xi_1\xi_2 + \eta^2}{\big((\xi-\xi_1)^2+\eta^2\big)\big((\xi-\xi_2)^2+\eta^2\big)} = \frac{4\pi\eta}{(\xi_1-\xi_2)^2+4\eta^2} < \infty$$

and tends to zero for vanishing η. Nonetheless, we would like not to neglect this term as it contains information about the interference between two paths as described in foregoing text. We rewrite this cross term in a more appealing way

$$\begin{aligned} &\frac{\xi^2 - (\xi_1+\xi_2)\xi + \xi_1\xi_2 + \eta^2}{\big((\xi-\xi_1)^2+\eta^2\big)\big((\xi-\xi_2)^2+\eta^2\big)} = \\ &\qquad = \frac{\xi_1-\xi_2}{(\xi_1-\xi_2)^2+4\eta^2} \left(\frac{\xi-\xi_1+\frac{2\eta^2}{\xi_1-\xi_2}}{(\xi-\xi_1)^2+\eta^2} - \frac{\xi-\xi_2+\frac{2\eta^2}{\xi_2-\xi_1}}{(\xi-\xi_2)^2+\eta^2} \right). \end{aligned} \tag{1.77}$$

Now, each fraction in the parentheses is suitable for regularization procedure, Eq. (1.68), if we define

$$\int d\xi \frac{g(\xi)}{(\xi-\xi_1)^2+\eta^2} \equiv \int_{-\infty}^{\infty} d\xi \frac{\xi-\xi_1+\frac{2\eta^2}{\xi_1-\xi_2}}{(\xi-\xi_1)^2+\eta^2} \big(n(\xi-\mu_i) - n(\xi-\mu_j)\big), \tag{1.78}$$

where $g(\xi) \equiv (\xi - \xi_1 + \frac{2\eta^2}{\xi_1-\xi_2})f(\xi)$. For $\eta \to 0^+$ we recover the components of the interference term in Eq. (1.74), which are replaced by regularized formula with digamma functions $\Psi_0(z)$

$$\int_{-\infty}^{\infty} \frac{d\xi}{\xi-\xi_1}\big(n(\xi-\mu_i)-n(\xi-\mu_j)\big) \\ \longrightarrow \Re\Big[\Psi_0\Big(\frac{1}{2}-\frac{\beta}{2\pi i}(\xi_1-\mu_j)\Big)-\Psi_0\Big(\frac{1}{2}-\frac{\beta}{2\pi i}(\xi_1-\mu_i)\Big)\Big]. \tag{1.79}$$

Hence, the inelastic paired current, linear in Fermi functions becomes

$$\begin{aligned} J_{ij}^{(\sigma),lin} = -\frac{e}{h}\Gamma_i^0\Gamma_j^0\Re\Big[&\frac{\beta}{2\pi i}\big(\Psi_1(\epsilon_{\bar\sigma},\mu_i)-\Psi_1(\epsilon_{\bar\sigma},\mu_j)\big) \\ &+\frac{\beta}{2\pi i}\big(\Psi_1(\epsilon_{\bar\sigma}+U,\mu_i)-\Psi_1(\epsilon_{\bar\sigma}+U,\mu_j)\big) \\ &+\frac{2}{U}\big(\Psi_0(\epsilon_{\bar\sigma},\mu_i)-\Psi_0(\epsilon_{\bar\sigma},\mu_j)\big) \\ &-\frac{2}{U}\big(\Psi_0(\epsilon_{\bar\sigma}+U,\mu_i)+\Psi_0(\epsilon_{\bar\sigma}+U,\mu_j)\big)\Big] \end{aligned} \tag{1.80}$$

with a proper limit of noninteracting particles, $\lim_{U\to 0} J_{ij}^{(\sigma),lin} = 0$.

There is one more point lacking our attention. A parameter η was incorporated into our theory somehow artificially. Despite that fact, it appears that it has clear physical meaning or at least this meaning could be restored. Consider a dot in the regime, where degenerate single electron state is most likely to be occupied so that $P_\uparrow = P_\downarrow = 1/2$. Hence, the current is given by Eq. (1.55), and in the vicinity of the peak, *i.e.* for $\xi = \epsilon_\sigma$, we are justified to neglect the contribution from the second fraction as it is much smaller than the first one. For this simplified expression we perform the regularization procedure according to Eq. (1.68) and write down the current through junction i in terms of this divergent part

$$J_i^{reg} = \sum_\sigma P_\sigma \sum_j J_{ij}^{(\sigma)} = -\frac{\pi}{\eta}\frac{e}{h}\Gamma_i^0 \sum_j \Gamma_j^0\big(n(\epsilon_0-\mu_i)-n(\epsilon_0-\mu_j)\big), \tag{1.81}$$

where we put $\epsilon_0 = \epsilon_\uparrow = \epsilon_\downarrow$ because of degeneracy. On the other hand, the current through a degenerate single electron state was derived in the sequential tunneling limit, Eq. (1.25) in Sec. 1.3.1

$$J_i = -\frac{2e}{\hbar}\frac{\Gamma_i^0\sum_{j=1}^N \Gamma_j^0\big(n(\epsilon_0-\mu_j)-n(\epsilon_0-\mu_j)\big)}{\sum_{j=1}^N \Gamma_j^0\big(1+n(\epsilon_0-\mu_j)\big)}. \tag{1.82}$$

Since this state is occupied, the Fermi functions in the denominator are approximately equal to unity, $n(\epsilon_0-\mu_i) = 1$. Comparing these two results, it becomes obvious that η has the interpretation of the dot level's width,

$2\eta = \sum_j \Gamma_j^0$. This broadening of the levels follows from the fact that the dot is not isolated system, but it is coupled to the outside world through the leads. This is a quite nice result that explicitly shows the correspondence between the two very different methods.

1.5 Exact results

The regime of noninteracting electrons gives possibility to compare the results we get within the framework of the second order perturbation theory with the exact result containing higher order terms in couplings. The quality of the cut off on the second order terms can be estimated. We will formulate the problem in two different formalisms and show that they lead to the same result. We end up with a discussion of the unpolarized leads case.

1.5.1 Resonant tunneling without correlations

Neglecting correlations, we start from the well-known result of Landauer [6] and Büttiker [7] describing the current through junction i in terms of a transmission coefficient $T_{ij}(\xi)$ and Fermi distribution functions of reservoirs

$$J_i = -\frac{e}{h}\int d\xi \sum_j T_{ij}(\xi)\big(n(\xi-\mu_j) - n(\xi-\mu_i)\big). \tag{1.83}$$

The transmission coefficient for an electron moving from lead j to lead i is

$$T_{ij}(\xi) = \mathrm{Tr}\big[G^A(\xi)\Gamma_i(\xi)G^R(\xi)\Gamma_j(\xi)\big] \tag{1.84}$$

with $\Gamma_j = i[\Sigma_j^R - \Sigma_j^A]$ describing a coupling of lead j to a quantum dot and the retarded (advanced) Green function given by

$$G^{R,A}(\epsilon) = \left[G_0^{-1} - \sum_j \Sigma_j^{R,A}(\epsilon)\right]^{-1}. \tag{1.85}$$

The free–particle Green function is

$$[G_0(\xi)]_{\sigma\sigma'} = \delta_{\sigma\sigma'}(\xi - \epsilon_\sigma)^{-1}, \tag{1.86}$$

while the retarded (advanced) self–energy $\Sigma_j^{R,A}$ follows from

$$[\Sigma_j^{R,A}(\xi)]_{\sigma\sigma'} = \sum_{k\sigma''}(R^\dagger)_{\sigma\sigma''}|t_{j,k\sigma''}|^2 g_{j,k\sigma''}^{R,A}(\xi)R_{\sigma''\sigma'} \tag{1.87}$$

for the polarized leads. Since derivation of the current for unpolarized leads is much simpler than in presence of polarization we will just give the final result for unpolarized leads afterwards. In the above formula $g_{j,k\sigma}^{R,A}(\xi)$ stands for the Green function of uncoupled leads

$$g_{j,k\sigma}^{R,A}(\xi) = (\xi - \xi_{j,k\sigma} \pm i0^+)^{-1}. \tag{1.88}$$

In order to simplify the analysis, we assume the wide band limit (the principal part integrates to zero then) and replace $g^{R,A}_{j,k\sigma}(\xi)$ by $\mp i\pi\delta(\xi - \xi_{j,k\sigma})$. Furthermore, we assume the tunneling width functions Γ_j are constant in energy. With these assumptions the couplings are

$$\mathbf{\Gamma}_j = \frac{1}{2}\Gamma^0_j \begin{pmatrix} 1 + P_j \cos\phi & P_j \sin\phi \\ P_j \sin\phi & 1 - P_j \cos\phi \end{pmatrix}, \tag{1.89}$$

where

$$\Gamma^0_j = 2\pi \sum_{k\sigma} |t_{j,k\sigma}|^2 \delta(\xi - \xi_{j,k\sigma}) = \sum_{\sigma} \Gamma^0_{j\sigma} \tag{1.90}$$

and P_j denotes the polarization of the tunneling from lead j defined as

$$\Gamma^0_{j\sigma} \equiv \frac{1}{2}(1 + \sigma\ P_j)\Gamma^0_j. \tag{1.91}$$

The polarization P_j may take three values; $P_j = 1$ for completely polarized lead with spin up electrons, $P_j = -1$ for leads polarized in the opposite direction and therefore coupling to spin down electrons only, and unpolarized lead with $P_j = 0$.

It is convenient to express $G^{R,A}(\epsilon)$ in terms of the free–particle Green function and the couplings Γ_j

$$G^{R,A}(\epsilon) = \Big[[G^{R,A}_0(\epsilon)]^{-1} \pm \frac{1}{2i} \sum_j \Gamma_j\Big]^{-1}. \tag{1.92}$$

The above equality holds because the retarded and advanced self–energies are not independent and satisfy the relation

$$[\Sigma^R_j]_{\sigma\sigma'} = \pi \sum_{k\sigma''} (R^\dagger)_{\sigma\sigma''} |t_{j,k\sigma''}|^2 \delta(\epsilon - \xi_{j,k\sigma''}) R_{\sigma''\sigma'} = -[\Sigma^A_j]_{\sigma\sigma'}. \tag{1.93}$$

On the other hand the couplings Γ_j relate to these self–energies via $\Gamma_j = i[\Sigma^R_j - \Sigma^A_j]$ and using the equality we just proved we end up with

$$\Gamma_j = 2i\Sigma^R_j = -2i\Sigma^A_j, \tag{1.94}$$

so that

$$\sum_j \Sigma^{R,A}_j(\epsilon) = \pm\frac{1}{2i} \sum_j \Gamma_j. \tag{1.95}$$

The derivation of the current in electrode i from Eqs. (1.83) and (1.84) is now straightforward. For unpolarized leads, $P_i = 0$,

$$J_i = -\frac{e}{h}\Gamma_i \sum_j \sum_\sigma \Gamma_j \int d\xi \frac{1}{\left(\xi - \epsilon_\sigma\right)^2 + \left(\frac{\Gamma}{2}\right)^2} \big(n(\xi - \mu_i) - n(\xi - \mu_j)\big) \tag{1.96}$$

with $\Gamma = \sum_i \Gamma_i$. This results agrees with one derived from the generalized Meir–Wingreen formula, and can be integrated analytically. Both topics will be discussed in the next paragraph.

1.5.2 Generalization of Meir–Wingreen formula

The result of Meir and Wingreen [8] for the current through an interacting electron region is well-known and being widely applied. The noninteracting Landauer–Bütticker formula for any number of leads is apparently not enough if one demands a high calculational precision. In the following paragraph we derive the generalization of the Meir–Wingreen formula that will include the indefinite number of leads and calculate the current J_i through one of the junctions.

We start from Kirchhoff's law

$$J_i + \sum_{\substack{j=1\\ j\neq i}}^{N} J_j = 0 \tag{1.97}$$

that leads to the obvious identity

$$J_i = \gamma\ J_i - (1-\gamma) \sum_{\substack{j=1\\ j\neq i}}^{N} J_j. \tag{1.98}$$

The main result of Meir and Wingreen is the current through lead i in presence of interactions

$$J_i = \frac{ie}{h} \int d\xi \Big\{ \mathrm{Tr}\big[\Gamma_i (G^R - G^A)\big] n(\xi - \mu_i) + \mathrm{Tr}\big[\Gamma_i G^<\big] \Big\}. \tag{1.99}$$

The above formula can be written in a bit different way employing Eq. (1.98)

$$\begin{aligned} J_i = \frac{ie}{h} \int d\xi \Big\{ &\gamma \Big(\mathrm{Tr}\big[\Gamma_i (G^R - G^A)\big] n(\xi - \mu_i) + \mathrm{Tr}\big[\Gamma_i G^<\big] \Big) \\ -(1-\gamma) &\sum_{\substack{j=1\\ j\neq i}}^{N} \Big(\mathrm{Tr}\big[\Gamma_j (G^R - G^A)\big] n(\xi - \mu_j) + \mathrm{Tr}\big[\Gamma_j G^<\big] \Big) \Big\}. \end{aligned} \tag{1.100}$$

The whole trick is to eliminate the lesser Green function, $G^<$. Providing all the couplings are proportionate, that is $\Gamma_i = \lambda_{ij} \Gamma_j$ where λ_{ij} are constants, we are allowed to move the parameter γ under the trace and manipulate it in such a manner that the term $\gamma \Gamma_i - (1-\gamma) \sum_{j=1,\ j\neq i}^{N} \Gamma_j$ in front of $G^<$

vanishes. Solving this equation with respect to γ and substituting the result into Eq. (1.100) we can show that

$$J_j = -\frac{e}{h}\int d\xi \sum_{i=1}^{N} \mathrm{Tr}\left[A\frac{\Gamma_j\Gamma_i}{\Gamma}\right]\big(n(\xi-\mu_i) - n(\xi-\mu_j)\big) \tag{1.101}$$

where we introduced a shorthand notation $\Gamma \equiv \sum_i \Gamma_i$ and wrote a formula for the current J_j in terms of the spectral function $A \equiv i(G^R - G^A)$.

One may prove (see for instance [2]) that the spectral function for a single level quantum dot is

$$A(\xi,\sigma) = \frac{\big(1-\langle n_{\bar\sigma}\rangle\big)\Gamma}{\big(\xi-\epsilon_\sigma\big)^2 + \big(\frac{\Gamma}{2}\big)^2} + \frac{\langle n_{\bar\sigma}\rangle\Gamma}{\big(\xi-\epsilon_\sigma-U\big)^2 + \big(\frac{\Gamma}{2}\big)^2}, \tag{1.102}$$

where Γ responds for the broadening of energy level due to the interactions with the leads. The limit of noninteracting electrons is solvable analytically, since unknown occupation numbers $\langle n_{\bar\sigma}\rangle$ cancel one another for $U = 0$ and a spin dependent spectral function becomes then

$$A(\xi,\sigma) = \frac{\Gamma}{\big(\xi-\epsilon_\sigma\big)^2 + \big(\frac{\Gamma}{2}\big)^2} \tag{1.103}$$

which substituted to the generalized Meir-Wingreen formula gives the exact current in lead i for a multiterminal device, valid to any order in couplings

$$J_i = -\frac{e}{h}\Gamma_i \sum_j \sum_\sigma \Gamma_j \int d\xi \frac{1}{\big(\xi-\epsilon_\sigma\big)^2 + \big(\frac{\Gamma}{2}\big)^2}\big(n(\xi-\mu_i) - n(\xi-\mu_j)\big) \tag{1.104}$$

We rewrite an integral that appears in J_s in more general form

$$\begin{aligned}\int_{-\infty}^{\infty} d\xi \frac{1}{\big(\xi-\epsilon_\sigma\big)^2 + \big(\frac{\Gamma}{2}\big)^2}\big(n(\xi-\mu_i) - n(\xi-\mu_j)\big)&\\ = -\frac{4}{\Gamma}\Im\int_{-\infty}^{\infty} \frac{1}{\xi-\epsilon_\sigma+i\frac{\Gamma}{2}}\big(n(\xi-\mu_i) - n(\xi-\mu_j)\big)&\end{aligned} \tag{1.105}$$

which can be calculated repeating the same procedure as described in App. A, with a small exception that is one must keep the imaginary term instead of taking the limit $\Gamma \to 0$. Finally, the current through junction i reads

$$J_i = -\frac{4e}{h}\Gamma_i \sum_j \sum_\sigma \Gamma_j \Im\Big[\Psi_0(\epsilon_\sigma,\mu_i,\Gamma) - \Psi_0(\epsilon_\sigma,\mu_j,\Gamma)\Big], \tag{1.106}$$

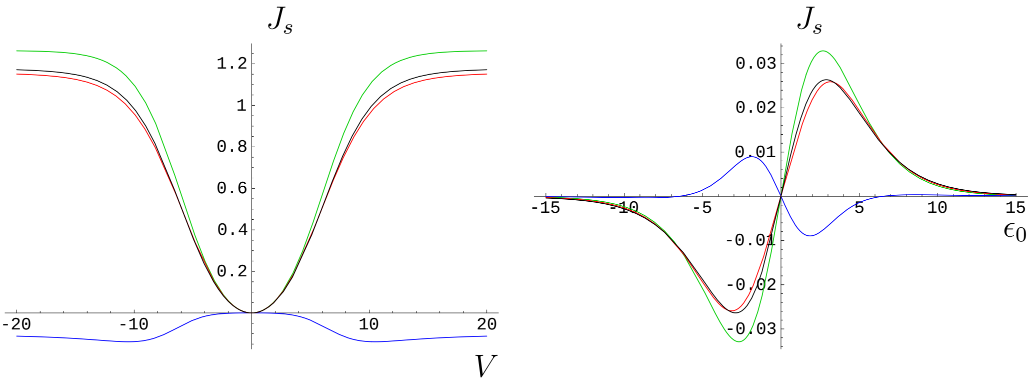

Figure 1.6: The comparison of the exact result given by Meir-Wingreen formula (in black) and the total stem current up to second order in couplings (the red curve). The sequential contribution is shown in green while the cotunneling part in blue. Here $\Gamma_l = \Gamma_r = \Gamma_s = \Gamma/3$, $k_B T = \Gamma/2$, $U = 0$, $B = 0$, $\epsilon_0 = 6$ on the left and $V = 1$ on the right.

where

$$\Psi_0(\epsilon_0, \mu, \Gamma) \equiv \Psi_0\Big(\frac{1}{2} - \frac{\beta}{2\pi i}(\epsilon_0 - \mu) + \frac{\beta}{4\pi}\Gamma\Big) \tag{1.107}$$

with $\Gamma = \Gamma_s + \Gamma_l + \Gamma_r$. This expression explicitly depends on Γ up to any order. It is advantageous to compare this exact result with a sum of the sequential current and the regularized cotunneling correction.

The three-terminal device was analyzed in detail for unpolarized leads. Therefore we confront the perturbative result with the exact one. We assume equal coupling to all leads, $\Gamma_l = \Gamma_r = \Gamma_s$ and the symmetrical biasing between the left lead $\mu_l = V$ and the right lead $\mu_r = -V$ with respect to the chemical potential of the central branch $\mu_s = 0$. The stem current in function of bias and the gate voltage is sketched in Fig. (1.6) for zero magnetic field, and for the magnetic field $B = 5$ in Fig. (1.7). These plots assure us that the second order perturbation theory gives is sufficient to get not only quantitative description, reachable also within the sequential tunneling framework, but also good qualitative estimation, at least for noninteracting electrons. The perturbative treatment is justified as long as $\Gamma < k_B T$, which defines a range of parameters for which the perturbation expansion works, the higher order terms might be neglected. The higher temperature compared to couplings we consider, the better approximation of the total current we get. Because in realistic systems we deal with devices working at relatively high temperature of hundreds Kelvin, it seems reasonable to cut off the perturbation expansion on second order.

Analyzing the plots depicted on this and the next page we come to the following conclusions. The total current is increased by virtual cotunneling

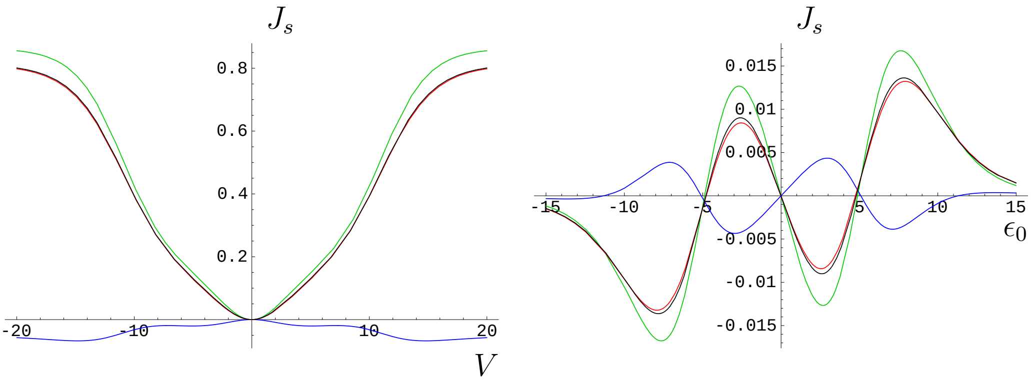

Figure 1.7: Similar comparison for noninteracting electrons, but with the external magnetic field $B = 5$. The other parameters are the same as in the previous plots.

processes for these values of gate voltage for which the sequential tunneling is exponentially suppressed. On the other hand the cotunneling correction lowers the sequential current maxima and gives rise to additional broadening of order $\Gamma_s + \Gamma_l + \Gamma_r$, so that the total broadening is now the sum of the thermal part and the latter.

Appendix A

Polygamma function

The polygamma function is a special function given by the n-th derivative of the digamma function $\Psi_0(z)$

$$\Psi_n(z) \equiv \frac{d^n}{dz^n}\Psi_0(z) = (-1)^n n! \sum_{k=0}^{\infty} \frac{1}{(z+k)^{n+1}}, \tag{A.1}$$

where digamma function $\psi_0(z)$ is defined as follows

$$\Psi_0(z) \equiv \frac{d}{dz}\ln\Gamma(z) = -\gamma - \sum_{k=0}^{\infty}\left(\frac{1}{k+z} - \frac{1}{k+1}\right) \tag{A.2}$$

with $\gamma = 0.57721\ldots$ being the so-called Euler-Mascheroni constant and $\Gamma(z)$ — the gamma function that is, in the Euler's integral form,

$$\Gamma_z \equiv \int_0^{\infty} t^{z-1}e^{-t}dt. \tag{A.3}$$

After this short introduction we can find the values of two integrals that appear in Sec. 1.4.2. First of all we will prove useful identity that allows us to extend integration along the real axis to the complex plain. Consider the Taylor expansion around the point $\xi = \xi_0$ of the following integral

$$\int d\xi \frac{f(\xi) - f(\xi_0)}{(\xi-\xi_0)^2 + \eta^2} = \int d\xi \frac{f'(\xi_0)(\xi-\xi_0) + \frac{1}{2}f''(\xi_0)(\xi-\xi_0)^2 + \ldots}{(\xi-\xi_0)^2+\eta^2}$$

and repeat the same for the expression

$$\begin{aligned}\frac{\partial}{\partial\xi_0}\Re\int d\xi \frac{f(\xi)}{\xi-\xi_0+i\eta} &= \Re\int d\xi\frac{f(\xi)}{(\xi-\xi_0+i\eta)^2} \\ &= \int d\xi \frac{(\xi-\xi_0)^2-\eta^2}{\left((\xi-\xi_0)^2+\eta^2\right)^2}\left(f(\xi_0) + f'(\xi_0)(\xi-\xi_0) + \frac{1}{2}f''(\xi_0)(\xi-\xi_0)^2 + \ldots\right)\end{aligned}$$

The first term integrated with $f(\xi_0)$ vanishes for any η. If we take the limit of $\eta \to 0^+$ in both cases then we find out that

$$\lim_{\eta\to 0^+} \int d\xi \frac{f(\xi) - f(\xi_0)}{(\xi-\xi_0)^2 + \eta^2} = \lim_{\eta\to 0^+} \frac{\partial}{\partial \xi_0} \Re \int d\xi \frac{f(\xi)}{\xi - \xi_0 + i\eta}. \tag{A.4}$$

As it has been already mentioned, there are two types of integrals that may contribute to the cotunneling current. We would like to find a similar identity for integrals of the second type

$$\lim_{\eta\to 0^+} \int d\xi \frac{g(\xi) - g(\xi_1)}{(\xi-\xi_1)^2 + \eta^2} = \lim_{\eta\to 0^+} \Re \int d\xi \frac{f(\xi)}{\xi - \xi_1 + i\eta} \tag{A.5}$$

with $g(\xi) \equiv (\xi - \xi_1 + \frac{2\eta^2}{\xi_1 - \xi_2}) f(\xi)$. The difference between $g(\xi)$ and $g(\xi_1)$ can be expressed in the following way

$$\int d\xi \frac{g(\xi) - g(\xi_1)}{(\xi-\xi_1)^2 + \eta^2} = \int d\xi \frac{f(\xi)(\xi-\xi_1)}{(\xi-\xi_1)^2 + \eta^2} + \frac{2\eta^2}{\xi_1 - \xi_2} \int d\xi \frac{f(\xi) - f(\xi_1)}{(\xi-\xi_1)^2 + \eta^2}.$$

The first integral is exactly the right-hand side integral in Eq. (A.5) while the second one is finite, and hence, the second term, proportional to η^2, goes to zero in the limit of $\eta \to 0$. This finishes a proof.

To represent these integrals by special functions, we begin from the expression

$$\begin{aligned} &\int_{-\infty}^{\infty} \frac{d\xi}{\xi - \xi_1} \big(n(\xi - \mu_j) - n(\xi - \mu_i)\big) \\ &\longrightarrow \Re \int_{-\infty}^{\infty} \frac{d\xi}{\xi - \xi_1 + i0^+} \big(n(\xi - \mu_j) - n(\xi - \mu_i)\big) \end{aligned}$$

that after the change of variables $\xi \to \frac{1}{\beta}\zeta + \mu_i$ in the first integral and, similarly, in the second one (with μ_i replaced by μ_j) becomes

$$\Re \int_{-\infty}^{\infty} d\zeta \left(\frac{1}{\zeta - \beta(\xi_1 - \mu_j) + i0^+} - \frac{1}{\zeta - \beta(\xi_1 - \mu_i) + i0^+} \right) \frac{1}{e^{\zeta} + 1}.$$

This integrals can be done easily by choosing a contour in the lower complex plane and summing over all the residues so that

$$\begin{aligned} &\Re \sum_{k=0}^{\infty} \left(\frac{2\pi i}{2\pi i(k + \frac{1}{2}) - \beta(\xi_1 - \mu_j)} - \frac{2\pi i}{2\pi i(k + \frac{1}{2}) - \beta(\xi_1 - \mu_i)} \right) \\ &= \Re \Big[\Psi_0\Big(\frac{1}{2} - \frac{\beta}{2\pi i}(\xi_1 - \mu_i)\Big) - \Psi_0\Big(\frac{1}{2} - \frac{\beta}{2\pi i}(\xi_1 - \mu_j)\Big) \Big], \end{aligned}$$

and the final answer is

$$\int_{-\infty}^{\infty} \frac{d\xi}{\xi - \xi_1} \big(n(\xi - \mu_j) - n(\xi - \mu_i)\big) \\ \longrightarrow \Re\Big[\Psi_0\Big(\frac{1}{2} - \frac{\beta}{2\pi i}(\xi_1 - \mu_i)\Big) - \Psi_0\Big(\frac{1}{2} - \frac{\beta}{2\pi i}(\xi_1 - \mu_j)\Big)\Big]. \tag{A.6}$$

The second function we need is found by differentiation

$$\int_{-\infty}^{\infty} \frac{d\xi}{(\xi - \xi_1)^2} \big(n(\xi - \mu_j) - n(\xi - \mu_i)\big) \\ = \frac{\partial}{\partial \xi_1} \int_{-\infty}^{\infty} \frac{d\xi}{\xi - \xi_1} \big(n(\xi - \mu_j) - n(\xi - \mu_i)\big) \\ \longrightarrow \Re\bigg[\frac{\beta}{2\pi i}\bigg(\Psi_1\Big(\frac{1}{2} - \frac{\beta}{2\pi i}(\xi_1 - \mu_j)\Big) - \Psi_1\Big(\frac{1}{2} - \frac{\beta}{2\pi i}(\xi_1 - \mu_i)\Big)\bigg)\bigg]. \tag{A.7}$$

Appendix B

Derivation of Green functions

The knowledge of Green functions gives us an useful tool for determining various physical observables. Therefore we need a powerful method to determine them. There are several ways of tackling this problem. Here, we will make use of so-called equation of motion technique to calculate the Green functions, given without proof in Sec. (1.5.1). The basic idea underlying this method is to generate a series of coupled differential equations by differentiating the function a number of times.If these equations close, the problem is in principle solvable; otherwise, one needs to invoke physical arguments to truncate the set of equations in a reasonable fashion (i.e. by neglecting certain correlations).

The derivation of the equation of motion is well established in the literature and will be omitted. Consider the Hamiltonian $H = H_0 + H_{\text{int}}$ in basis $\{\nu\}$ with

$$H_0 = \sum_{\nu\nu'} t_{\nu\nu'} a_\nu^\dagger a_{\nu'} \tag{B.1}$$

and H_{int} standing for an interaction part. The equation of motion in energy domain is of the form

$$\sum_{\nu\nu'} \big(\delta_{\nu\nu''}(\epsilon + i0^+) - t_{\nu\nu''}\big) G^R(\nu'', \nu; \epsilon) = \delta_{\nu\nu'} + D^R(\nu, \nu'; \epsilon), \tag{B.2}$$

$$D^R(\nu, \nu'; \epsilon) = -i \int_{-\infty}^{\infty} dt e^{i(\epsilon + i\eta)(t-t')} \theta(t-t') \Big\langle \big\{ \{H_{\text{int}}, a_\nu\}(t), a_{\nu'}^\dagger(t') \big\} \Big\rangle. \tag{B.3}$$

The calculation of a free-particle Green function for the dot Hamiltonian Eq. (B.4) in the non-interacting case

$$H_D = \sum_\sigma (\epsilon_0 - \sigma B) \tilde{d}_\sigma^\dagger \tilde{d}_\sigma \tag{B.4}$$

is straightforward now

$$[G_0^R(\epsilon)]_{\sigma\sigma'} = \delta_{\sigma\sigma'}(\epsilon - \epsilon_0 + \sigma B + i0^+)^{-1}. \tag{B.5}$$

In the same way we find the Green function for the uncoupled leads.

The situation of the dot coupled to the leads is just a bit more complicated. The proper Hamiltonian Eq. (1.1) together with definitions of it counterparts was described in Sec. (1.2). We will find the equations of motion by letting ν and ν'' in Eq. (B.2) run over the lead states $j, k\sigma$ and the dot states σ. One should not confuse spin index numbering states in the leads and in the dot. We obtain coupled equations

$$(\epsilon + i0^+ - \epsilon_0 + \sigma B)G^R(\sigma, \sigma; \epsilon) - \sum_{j,k\sigma}\sum_{\sigma'} t_{j,k\sigma'} R_{\sigma'\sigma} G^R(j, k\sigma, \sigma; \epsilon) = 1 \tag{B.6}$$

$$(\epsilon + i0^+ - \xi_{j,k\sigma})G^R(j, k\sigma, \sigma; \epsilon) - \sum_{\sigma'} t^*_{j,k\sigma'} R^\dagger_{\sigma'\sigma} G^R(\sigma, \sigma; \epsilon) = 0 \tag{B.7}$$

The first bracket in the upper equation is equal to $[G_0^R]^{-1}$ whereas the first bracket in the second equation is just $[g^R_{j,k\sigma}]^{-1}$, hence

$$G^R(\epsilon) = \frac{1}{G_0^{-1}(\epsilon) - \sum_j \Sigma_j^R(\epsilon)} \tag{B.8}$$

with

$$[\Sigma_j^R(\epsilon)]_{\sigma\sigma'} = \sum_{k\sigma''} (R^\dagger)_{\sigma\sigma''} |t_{j,k\sigma''}|^2 g^R_{j,k\sigma''}(\epsilon) R_{\sigma''\sigma'}. \tag{B.9}$$

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