Quantum phase transition and conductivity of parallel quantum dots with a moderate Coulomb interaction

V S Protsenko[1,2]**, A A Katanin**[1,2]

[1] Institute of Metal Physics, Kovalevskaya str. 18, Ekaterinburg 620990, Russia
[2] Ural Federal University, Mira str. 19, Ekaterinburg 620002, Russia

E-mail: `protsenko.vladimir15@mail.ru`, `katanin@mail.ru`

Abstract. We study the effects of electronic interactions on transport through parallel quantum dots connected symmetrically to leads, focusing on the case of an intermediate value of the on–site Coulomb interaction at each quantum dot. We apply both the mean-field (MF) approximation and the functional renormalization group (fRG) approach with using the Litim regularization scheme in frequency space to treat the effect of interaction and calculate the energy levels, the magnetization, the square of local spin as well as the linear conductance as a function of gate voltage. Already for intermediate values of the Coulomb interaction, the system exhibits a quantum phase transition from the parallel aligned (high spin state) to the paramagnetic (low spin) regime. This phase transition is accompanied by the appearance of the step discontinuities in the conductance, which can be observed in the experiment.

1. Introduction

A quantum dot is formed by a nanostructure that restricts the motion of electrons in all three directions. The Coulomb interaction can play a crucial role in the electron transport through quantum dots. Even in the simplest system consisting of a single quantum dot at sufficiently low temperatures, the Coulomb interaction can lead to the Kondo plateau in the total conductance [1, 2].

Especially interesting cases are those in which electrons can pass through the mesoscopic system following different paths, which can result in quantum interference effects [3, 4]. In the article [5] within the numerical renormalization group [6] it has been shown that the strong Coulomb interaction in such geometries leads to the parallel spin alignment state as the ground state of the systems in some range of gate voltages. Moreover, it has been found that this phase transition is accompanied by the appearance of the resonance in conductance. On the other hand, in the non-interacting case the non-magnetic state is realized. Therefore, the problem of influence of the intermediate Coulomb interaction on the spin alignment and electron transport is not trivial.

In this paper, we consider the simplest ring configuration, namely parallel quantum dots connected to two common leads. We focus on the case of an intermediate value of the on-site Coulomb interaction U in each quantum dot, and introduce a weak magnetic field H. The local Coulomb interaction is treated within the functional renormalization group (fRG) approach [2, 7–9] with using the Litim regularization scheme [10]. As a result, via fRG we calculate the

energy levels, the magnetization, the square of local spin as well as the linear conductance as function of the gate voltage.

2. The model
The system of two quantum dots coupled in parallel, which are connected to common leads, can be described by the following Hamiltonian:

$$\mathcal{H} = \mathcal{H}_l + \mathcal{H}_d + \mathcal{H}_c. \tag{1}$$

Here $\mathcal{H}_l$ is the part of the Hamiltonian that describes the leads. We assume that the left and the right leads are equivalent and described by a non-interacting Hamiltonian. The next term in (1) is the Hamiltonian of the quantum dots:

$$\mathcal{H}_d = \sum_\sigma \sum_{j=1}^2 \epsilon_{j,\sigma} d^\dagger_{j,\sigma} d_{j,\sigma} + \sum_\sigma \sum_{j=1}^2 \frac{U_j}{2} \left(d^\dagger_{j,\sigma} d_{j,\sigma} - \frac{1}{2} \right) \left(d^\dagger_{j,\bar\sigma} d_{j,\bar\sigma} - \frac{1}{2} \right), \tag{2}$$

where $d^\dagger_{j,\sigma} (d_{j,\sigma})$ denote creation (annihilation) operators for an electron with spin $\sigma \in \{\uparrow, \downarrow\}$ localized on the j-th ($j \in \{1,2\}$) quantum dot. The index $\bar\sigma$ is the complement of σ ($\bar\sigma = \uparrow$ if $\sigma = \downarrow$ and vice versa). In general, each quantum dot level $\epsilon_{j,\sigma}$ consists of a constant part ϵ_j^0 and the part which includes the gate voltage V_g, as well as the magnetic field $\mathcal{H}$:

$$\epsilon_{j,\sigma} = \epsilon_j^0 + V_g - \sigma \frac{\mathcal{H}}{2}. \tag{3}$$

Therefore, the level positions can be shifted by applying a gate voltage or a magnetic field. The second term in $\mathcal{H}_d$ accounts for the two–particle interaction between electrons, where the parameter U_j is the on–site Coulomb repulsion of spin up and down electrons. Finally, the last terms in $\mathcal{H}$ take into account the coupling between dots and leads. It is given by:

$$\mathcal{H}_c = -\sum_\sigma \sum_{l=L,R} \sum_j (t_j^l c^\dagger_{0,\sigma,l} d_{j,\sigma} + \text{H.c.}), \tag{4}$$

with leads creation (annihilation) operators $c^\dagger_{0,\sigma,l}$ ($c_{0,\sigma,l}$) for an electron with spin direction σ on the first lattice site of the left or right lead (l=L or l=R respectively). Here t_j^l is the tunnel matrix element between a lead l and a quantum dot j.

In this paper we focus on the symmetric coupling case with equal local interaction $U_j = U$ ($j \in \{1,2\}$) in quantum dots. In this case, the inverse of the noninteracting propagator reads as [2]

$$\mathcal{G}_0^{-1}(i\omega, \sigma) = \begin{pmatrix} i\omega - V_g + \sigma \dfrac{H}{2} + i\dfrac{\Gamma}{2} \operatorname{sgn}(w) & i\dfrac{\Gamma}{2} \operatorname{sgn}(w) \\ i\dfrac{\Gamma}{2} \operatorname{sgn}(w) & i\omega - V_g + \sigma \dfrac{H}{2} + i\dfrac{\Gamma}{2} \operatorname{sgn}(w) \end{pmatrix}, \tag{5}$$

where we have introduced the frequency independent hybridization function

$$\Gamma = \sum_{j,l} \Gamma_j^l = \pi \sum_{j,l} |t_j^l|^2 \rho_{lead}, \tag{6}$$

ρ_{lead} is the local density of states of the leads at the quantum dot site 0.

The full Green function $\mathcal{G}$ is given by the Dyson equation $\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \Sigma$, where Σ is a self-energy of the system.

3. The method

In this section we will briefly review the recently proposed method of the functional renormalization group [2, 7-9, 11]. It inherits the basic ideas of the Wilsonian RG [12] and allows to express the Wilson mode elimination in terms of an exact functional differential equation for the generating functionals.

In our case, primary quantities of interest are the irreducible vertex functions. More precisely, we are mainly interested in the self-energy (one–particle vertex), since it allows us to obtain directly the Green function of the interacting quantum dots system in the presence of the contacts, which is our main goal. The one–particle irreducible (1PI) scheme [8] is a suitable choice for this purpose. The RG equations in the 1PI scheme are obtained by inserting $\mathcal{G}_0(\Lambda)$ in the generating functional of the one-particle irreducible vertex functions. An infinite hierarchy of differential equations for 1PI vertex functions is obtained by taking the derivative of generating functional with respect to Λ and then expanding it in powers of the external fields.

We write down the explicit equations for the first two vertex functions, namely for the self–energy (one-particle vertex) Σ^Λ:

$$\partial_\Lambda \Sigma^\Lambda(k';k) = -\sum_{q'q} e^{i\omega_2 0^+} \mathcal{S}^\Lambda(q,q')\Gamma_4^\Lambda(k',q';k,q) \tag{7}$$

and the effective two-particle interactions (two-particle vertex) Γ^Λ:

$$\begin{aligned}
\partial_\Lambda \Gamma_4^\Lambda(k_1',k_2';k_1,k_2) = \sum_{s,s',q,q'} & \mathcal{G}^\Lambda(s,s')\mathcal{S}^\Lambda(q,q') \\
\times & \Big\{ \Gamma_4^\Lambda(k_1',k_2';s,q)\Gamma_4^\Lambda(s',q';k_1,k_2) \\
& - \Big[\Gamma_4^\Lambda(k_1',q';k_1,s)\Gamma_4^\Lambda(s',k_2';q,k_2) + (s \leftrightarrows q, s' \leftrightarrows q') \Big] \\
& + \Big[\Gamma_4^\Lambda(k_2',q';k_1,s)\Gamma_4^\Lambda(s',k_1';q,k_2) + (s \leftrightarrows q, s' \leftrightarrows q') \Big] \Big\} \\
& - \sum_{k,k'} \mathcal{S}^\Lambda(k,k')\Gamma_6^\Lambda(k_1',k_2',k';k_1,k_2,k),
\end{aligned} \tag{8}$$

where the indices $k_i(k_i')$ collect all quantum numbers (in our case they are dot indices $\{i,j\ldots\}$, frequencies w, and spin indices σ) and $\mathcal{S}^\Lambda$ denotes the so-called single-scale propagator:

$$\mathcal{S}^\Lambda = \mathcal{G}^\Lambda \partial_\Lambda \left(\mathcal{G}_0^\Lambda\right)^{-1} \mathcal{G}^\Lambda. \tag{9}$$

In order to solve this infinite set of coupled differential equations, it must be truncated in some manner. For this, in the following, we completely neglect the flow of the vertex functions Γ_{2m}^Λ for $m \geqslant 3$. Thus, the three-particle contributions Γ_6^Λ vanish and we have a closed system of the RG equations for Σ^Λ and Γ_4^Λ.

Now we need to specify the explicit dependence of the $\mathcal{G}_0^\Lambda$ on parameter Λ, which will be used in our calculations. It is important because due to the truncation of the infinite hierarchy of RG equations different cutoff schemes are not equivalent. For this reason, an incorrect choice of the cutoff can lead to unphysical divergences of the vertex functions. For example, it was noted that the most frequently used cutoff function – sharp multiplicative cutoff may lead to unphysical behavior of the vertex functions.

In order to avoid this problem, in this article we introduce another regularization method for bare propagator, namely

$$\left[\mathcal{G}_0^\Lambda\right]^{-1} = [\mathcal{G}_0]^{-1} + i\left(\Lambda - |\omega_n|\right)\Theta\left(\Lambda - |\omega_n|\right)\operatorname{sgn}(\omega_n), \tag{10}$$

which is analogous to proposed by Litim [10]. This smooth additive cutoff has the undoubted advantage, compared with sharp cutoff, since it smoothly switched off the propagator at low frequencies.

4. Results and discussion

At first we consider the effect of the intermediate electron–electron interactions on the position of the energy levels $\epsilon_{j\sigma} = V_g - \sigma\dfrac{H}{2} + \Sigma_j^\sigma$, where the self-energy Σ can be extracted from the functional renormalization group calculations. These quantities are important because their position relative to the Fermi level greatly determines the conductivity of the system. Note that due to the symmetry of the system, $\epsilon_{1\sigma} = \epsilon_{2\sigma}$. In figure 1 (a) the energy levels of quantum dots $\epsilon_{j\sigma}$ are plotted as a function of the gate voltage V_g. There are two major regions of the gate voltage in which energy levels are split differently.

For $|V_g| > |V_g^c|$ the energy difference between spin up and spin down states is of the order of magnitude of the applied field H. This results in the difference between the average occupation numbers of spin up and down electrons which is also proportional to the magnetic field. One
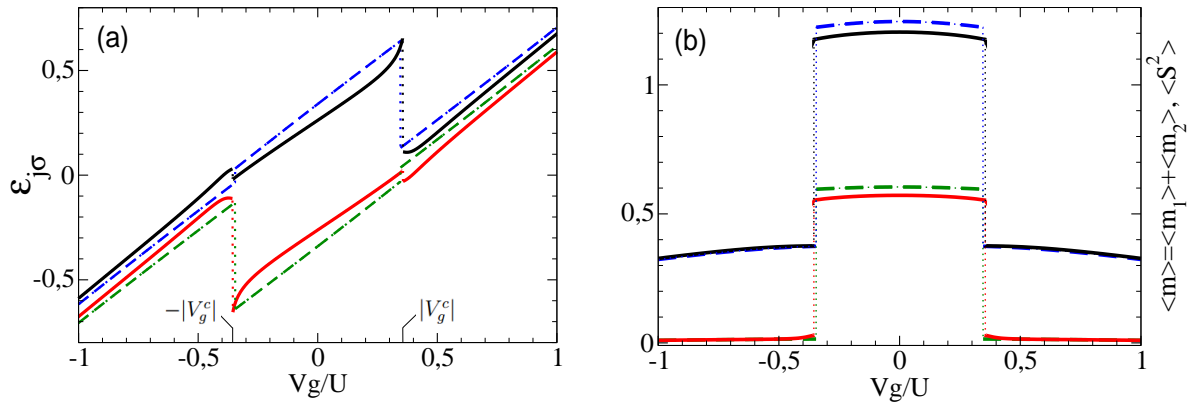

Figure 1. (a) The energy levels $\epsilon_{j\sigma}$ as a function of the gate voltage. Solid up (down) line: $\epsilon_{j\downarrow}$ ($\epsilon_{j\uparrow}$) in the fRG. Dashed up (down) line: $\epsilon_{j\downarrow}$ ($\epsilon_{j\uparrow}$) in the MF. (b) Gate voltage dependence of the average of the square of the total spin $\langle \mathbf{S}^2 \rangle$ and the total magnetization $m = m_1 + m_2$. Upper solid (black) line: $\langle \mathbf{S}^2 \rangle$ in the fRG. Upper dashed (blue) line: $\langle \mathbf{S}^2 \rangle$ in the MF. Lower solid (red) line: m in the fRG. Lower dashed (green) line: m in the MF. The parameters are $U/\Gamma = 1$ and $H/U = 0.08$.

can see that this energy level splitting increases with decreasing the gate voltage up to $|V_g^c|$. Consequently, magnetization $m_j = \dfrac{1}{2}(\langle n_{j\uparrow} \rangle - \langle n_{j\downarrow} \rangle)$ on each quantum dot begins to grow for $|V_g| \to |V_g^c|$ (figure 1 (b)).

In the range of voltages $|V_g| < |V_g^c|$ the Coulomb interaction leads to the strong splitting of the $\epsilon_{j\uparrow}$ and $\epsilon_{j\downarrow}$ energy levels in an external magnetic field. Now, the energy of the spin up state is much lower than that of the spin down state. Therefore, the occupancy of the spin-up state becomes energetically favoured over the spin-down state. This results in $0 < m_j \sim 1$, $\langle \mathbf{S}^2 \rangle \sim 1$ and a formation of a high spin state on each quantum dot. In this case the RG calculation predicts a very weakly expressed decrease in both the magnetization and the average of the square of the total spin for $|V_g| \to |V_g^c|$.

At the point $|V_g| = |V_g^c|$, when the above two regimes change into one another, the phase transition take place and all the discussed above physical quantities show the jump behavior.

Figure 1 shows the gate voltage dependence of the average of the square of the total spin $\langle \mathbf{S}^2 \rangle$. It shows a sharp increase in $\langle \mathbf{S}^2 \rangle$ as $|V_g|$ falls below $|V_g^c|$. That is a direct indication of the phase transition. Thus, accounting for the intermediate value of the interaction enables us to conclude that in this case we have the same type of phase transition as in the case of the strong Coulomb interaction in quantum dots. Comparison between fRG and mean-field approximation depicted in figure 1 shows qualitative agreement. In the mean-field approximation the phase transition is also accompanied by a jump–like change of the occupation number and the energy of levels. But, one sees that the results of the two methods lead to the different behavior of the curves of the energy levels, as well as the different estimates of the square of the total spin $\langle \mathbf{S}^2 \rangle$ and the total magnetization m for voltage V_g near half-filling.

Knowing the renormalized energy levels and renormalization of the hopping parameter allows us to calculate the quantity of our main interest: the linear-response conductance G as a function of the gate voltage. For the present setup, the linear conductance $G = dI/dV_{sd}$ of an interacting system can be computed as [2]:

$$G = G_0 \frac{\Gamma^2}{8} \sum_\sigma \left| \sum_{j,j'} \mathcal{G}_{j,j'}^\sigma(0) \right|^2, \tag{11}$$

where $G_0 = \dfrac{2e^2}{h}$ is the conductance quantum.

First we consider the non-interacting case, $U = 0$. After replacing $\mathcal{G} \to \mathcal{G}_0$ in (11) we have:

$$G(V_g) = \frac{e^2}{h} \sum_\sigma G_\sigma(V_g) = \frac{e^2}{h} \sum_\sigma \frac{\Gamma^2}{\left(V_g - \sigma \dfrac{H}{2} \right)^2 + \Gamma^2}, \tag{12}$$

which is a superposition of two Lorentzians with peak positions at $V_g = \sigma \dfrac{H}{2}$.

If we include the interaction between spin up and spin down electrons on both quantum dots, the transport properties of the system changes greatly. Even at the level of mean field
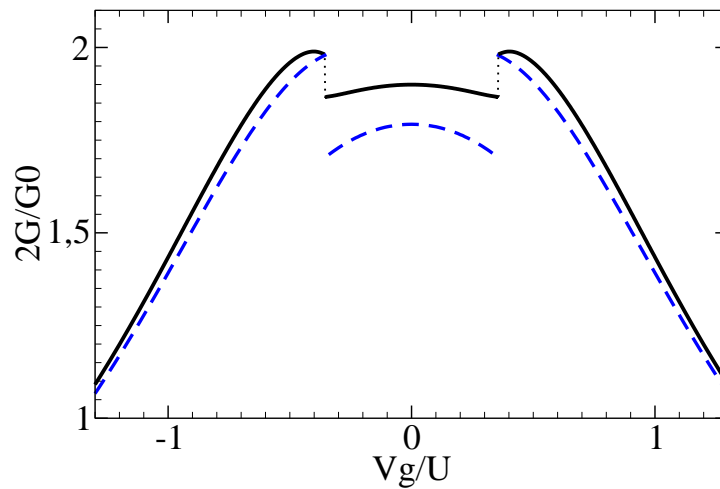

Figure 2. Conductance $2G/G_0$ as a function of V_g/U of the parallel double dot with $U = \Gamma$ and $H = 0.08U$. Solid black line: fRG approach with the Litim cutoff. Dashed blue line: MF approximation.

approximation, the dependence of the conductance on the gate voltage changes its lineshape, the transition between the phases of the different spin symmetries is accompanied by a jump in the conductance (figure 2). We also observe a sharp drop of the conductance in the high spin state. These features of the $G(V_g)$ can be explained via the position of the double quantum dots system energy levels with respect to the Fermi level.

Next, we calculate the gate voltage dependence of the linear conductance using the functional renormalization group scheme. As shown in figure 2, the phase transition is manifested by the appearance of the step discontinuities in the curve of the conductance. Importantly, the drop of the conductance in the high spin state is smaller than in the case of the mean-field approach. Furthermore, even in the low spin (paramagnetic) regime one can see a notable difference in the linear conductance. In this case, the fRG gives higher value of the conductivity at the same gate voltage. We also note that in this case, the conductivity is not completely determined by the position of the $\epsilon_{j\sigma}$ levels. This is due to the fact that the off-diagonal components of the self-energy are also renormalized in a non trivial way. They have a two-fold effect on the conductivity: modify renormalization of $\epsilon_{j\sigma}$ (and vice versa) and explicitly enter into the expression for $G(V_g)$. Thus, the individual contributions of the self-energy to the conductivity are mixed in the obtained results.

5. Conclusion

We found that in the case of an intermediate value of the on-site Coulomb interaction the fRG with the Litim cutoff reproduce correlation effects. The system exhibits a quantum phase transition between the high spin state and a low spin state that is driven by the gate voltage. This phase transition is accompanied by the appearance of the step discontinuities in the conductance, which can be observed in the experiment. In the phase transition region, the magnetization and the energy of levels of the quantum dots computed in the fRG also show a jump–like behavior.

Comparison between fRG and mean-field approximation shows that although they are in qualitative agreement and give the same estimate for the gate voltage of the phase transition, they yield to significantly different behavior of conduction and other considered variables in the spin ordered phase.

References
[1] Andergassen S, Enss T and Meden V 2006 *Phys. Rev.* B **73** 153308
[2] Karrasch C, Enss T and Meden V 2006 *Phys. Rev.* B **73** 235337
[3] Orellana P A, Ladrón de Guevara M L and Claro F 2004 *Phys. Rev.* B **70** 233315
[4] Ladrón de Guevara M L, Claro F and Orellana P A 2003 *Phys. Rev.* B **67** 195335
[5] Zitko R and Bonca J 2007 *Phys. Rev.* B **76** 241305(R)
[6] Bulla R, Costi T and Pruschke T 2008 *Rev. Mod. Phys.* **80** 395
[7] Wetterich C 1993 *Phys. Lett.* B **301** 90
[8] Salmhofer M and Honerkamp C 2001 *Prog. Theor. Phys.* **105** 1
[9] Salmhofer M 1999 *Renormalization* (Berlin: Springer)
[10] Litim D F 2001 *Phys. Rev.* D **64** 105007
[11] Salmhofer M, Honerkamp C, Metzner W, and Lauscher O 2004 *Phys. Rev.* B **112** 943
[12] Wilson K G 1975 *Phys. Rev.* B **47** 773