Transport through a double quantum dot with interdot repulsion

Yunori Nisikawa and Akira Oguri
Department of Material Science, Osaka City University, 3-3-138 sumiyoshi-ku Osaka, Japan
E-mail: nisikawa@sci.osaka-cu.ac.jp

Abstract. We study transport through a double quantum dot with interdot hopping $t$, intradot repulsion $U$ and interdot repulsion $U'$, using the numerical renormalization group (NRG) method. At half-filling, the conductances in two-terminal series and four-terminal parallel configuration are calculated via two phase shifts for quasi-particles of double quantum dot connected to two noninteracting leads with hybridization strength $\Gamma$. For small values of $t/\Gamma$ and $U'/U$, conductance in the two-terminal series configuration is suppressed to almost zero. In this region, plateau of conductance in the four-terminal parallel configuration appears and almost reaches a unitary limit value $4e^2/h$ of two conducting modes. For large values of $t/\Gamma$ or $U'/U$, both conductances are suppressed to almost zero. The conductance in the two-terminal series configuration almost reaches a unitary limit value $2e^2/h$ only around crossover regions of electron-configuration in double quantum dot. Through the behavior of the local charge and some thermodynamic quantities, we discuss the relation between transport and electron-configuration.

A half-filled double quantum dot with interdot repulsion has been theoretically studied [1, 2, 3] and some interesting phenomena, for example, quantum phase transition at a critical interdot repulsion [1], have been predicted. In this paper, focusing on two kind of conductance through a half-filled double quantum dot with interdot repulsion, we discuss the relation between transport and electron-configuration of double quantum dot through the behavior of the local charge and some thermodynamic quantities, on the basis of numerical renormalization group (NRG) calculation.

We consider two-site Hubbard model with interdot repulsion, which is connected to two non-interacting leads at the left(L) and right(R) by the symmetrical tunneling matrix elements $v$, as illustrated in Fig.1 (a).

The Hamiltonian is given by $H = H_D + H_{\text{mix}} + H_{\text{lead}}$ with

$$H_D = \epsilon_d \sum_{\sigma} d_{1\sigma}^\dagger d_{1\sigma} - t \sum_{\sigma} \left( d_{1\sigma}^\dagger d_{2\sigma} + d_{2\sigma}^\dagger d_{1\sigma} \right) + U \sum_{\sigma} d_{1\uparrow}^\dagger d_{1\downarrow} d_{1\downarrow}^\dagger d_{1\uparrow},$$

$$H_{\text{mix}} = v \sum_{\sigma} \left( d_{1\sigma}^\dagger \psi_{L\sigma}^+ + \psi_{L\sigma}^+ d_{1\sigma} \right) + v \sum_{\sigma} \left( \psi_{R\sigma}^+ d_{2\sigma} + d_{2\sigma}^\dagger \psi_{R\sigma} \right),$$

$$H_{\text{lead}} = \sum_{\nu=L,R} \sum_{k\sigma} \epsilon_{k\nu} c_{k\nu\sigma}^\dagger c_{k\nu\sigma},$$

where $d_{1\sigma}$ and $d_{2\sigma}$ are the destruction operators of the double quantum dot, and $\psi_{L\sigma}$ and $\psi_{R\sigma}$ are the destruction operators of the left and right leads, respectively; $\epsilon_d$ is the energy of the double quantum dot, $t$ is the hopping integral, $U$ is the intradot repulsion, $U'$ is the interdot repulsion, $\Gamma$ is the hybridization strength, $v$ is the tunneling matrix element, and $\epsilon_{k\nu}$ is the energy of the $\nu$-th lead.
where \( d_{\sigma} \) annihilates an electron with spin \( \sigma \) at site \( i \) in the double quantum dot, which is characterized by the interdot hopping matrix element \( t \), onsite energy \( \epsilon_d \), intradot repulsion \( U \) and interdot repulsion \( U' \). In the lead at \( \nu \) \((= L, R)\), the operator \( c^\dagger_{k\nu\sigma} \) creates an electron with energy \( \epsilon_{k\nu} \) corresponding to an one-particle state \( \phi_{k\nu}(r) \). The linear combinations of the conduction electrons \( \psi_{L\sigma} \) and \( \psi_{R\sigma} \) mixed with the electrons in dots labeled by \( i = 1 \) and \( 2 \), respectively, where \( \psi_{i\nu\sigma} = \sum_k c_{k\nu\sigma} \phi_{k\nu}(r_{\nu}) \) and \( r_{\nu} \) is the position at the interface in the lead \( \nu \). We assume that the hybridization strength \( \Gamma \equiv \pi v^2 \sum_k |\phi_{k\nu}(r_{\nu})|^2 \delta(\omega - \epsilon_{k\nu}) \) is a constant independent of the frequency \( \omega \) and \( \nu \), and take the Fermi energy \( \mu \) to be \( \mu = 0 \).

Our system has an inversion symmetry, so we can introduce the even and odd-parity orbitals as follows:

\[
\begin{align*}
 a_\sigma &= \frac{d_{1\sigma} + d_{2\sigma}}{\sqrt{2}}, & b_\sigma &= \frac{d_{1\sigma} - d_{2\sigma}}{\sqrt{2}}. \\
\end{align*}
\]

Two phase shifts \( \delta_e \) and \( \delta_o \) of the quasi-particles with even and odd parities characterize a local Fermi-liquid behavior of the whole system described by \( H \) at low temperature. We can obtain \( \delta_e \) and \( \delta_o \) from the fixed-point eigen values of NRG. From two phase shifts defined with respect to the system described by \( H \), we can deduce not only the conductance \( g_s \) in the two-terminal series configuration illustrated in Fig. 1(a) but also the conductance \( g_p \) in four-terminal parallel configuration illustrated in Fig. 1(b) at \( T = 0 \) as follows:

\[
\begin{align*}
 g_s &= \frac{2e^2}{h} \sin^2(\delta_e - \delta_o), & g_p &= \frac{2e^2}{h} \left( \sin^2\delta_e + \sin^2\delta_o \right). \\
\end{align*}
\]

We calculate series conductance \( g_s \), parallel conductance \( g_p \), electron number \( n_e \equiv \sum_\sigma \langle a_{\sigma}^\dagger a_{\sigma} \rangle \) in even-parity orbital defined by Eq. (4) and some thermodynamic quantities at half-filling \( \epsilon_d = -U/2 - U' \) for \( 10^{-4} \leq t/\Gamma \leq 10 \) and \( 0 \leq U'/U \leq 1.5 \). In this paper, we fix \( U/\Gamma \) to be \( U/\Gamma = 15 \). In Fig. 2(a) \( g_s \), (b) \( g_p \) and (c) \( n_e \) are plotted as functions of \( t/\Gamma \) and \( U'/U \). First of all, to make discussion clear, we consider three limit case; case 1: \( t/\Gamma \to 0 \) and \( U'/U \to 0 \), case 2: \( t/\Gamma \to \infty \) and \( U'/U \to 0 \), and case 3: \( t/\Gamma \to 0 \) and \( U'/U \to \infty \). In Fig. 2(a), we illustrate schematic picture of electron-configuration in double quantum dot for these three limit cases. In the case 1, because of no interaction between two dots, our system is decoupled to two same systems composed of a single dot connected to a single lead. At half-filling, each single dot is occupied by one electron to avoid intradot repulsion \( U \), as shown in the picture [case 1] in Fig. 2(a). Schematic picture [case 2] in Fig. 2(a) represents that two electrons occupy the even-parity orbital stabilized by large interdot hopping \( t \) in the case 2. So, we can expect that the electronic states of the \( n_e \simeq 2 \) region in Fig. 2(c) are similar to the state of the case 2. The case 3 have been studied in detail by Galpin et al. using NRG [1][2]. Either of two dot is occupied by
two electrons to avoid strong interdot repulsion $U'$ which is much larger than intradot repulsion $U$, as shown in the picture [case 3] in Fig. 2(a). Therefore, a degenerate configuration of two electrons results in non-Fermi liquid ground state with ln2 residual entropy. From Fig. 2(a) and above discussion, we find that the series conductance $g_s$ almost reaches a unitary limit value $2e^2/h$ only around cross-over regions of electron-configuration in double quantum dot. Next, we discuss the parallel conductance $g_p$ in three limit cases. From the similar discussion for two-terminal series configuration, we can easily understand the schematic pictures of electron-configuration in four-terminal parallel configuration for three limit case, shown in Fig. 2(b). For the case 1, our system is decoupled to two same systems composed of single-dot connected to two leads. In each system, one electron occupies single dot as shown in the picture [case 1] in Fig. 2(b), and causes Kondo effect. Therefore, the parallel conductance $g_p$ reaches a unitary limit value equal to $4e^2/h$ of two conducting modes. From Fig. 2(b), we indeed find that there is plateau of the parallel conductance $g_p$, which almost reaches a unitary limit value $4e^2/h$, for small values of $t/\Gamma$ and $U'/U$. The even-parity bonding orbital of double-dot is fully occupied by the two electrons in the case 2. In the case 3, two electrons fully occupy either of two dots and no electron occupies the other, as shown in the picture [case 3] in Fig. 2(b). Therefore, the parallel conductance in both case 2 and 3 is 0. This corresponds to the fact that the parallel conductance for large values of $t/\Gamma$ or $U'/U$ is suppressed to almost zero, as shown in Fig. 2(b).

In summary, we have studied transport through a half-filled double quantum-dot with interdot repulsion $U'$ which is much larger than intradot repulsion $U$, as shown in the picture [case 3] in Fig. 2(a). Therefore, a degenerate configuration of two electrons results in non-Fermi liquid ground state with ln2 residual entropy. From Fig. 2(a) and above discussion, we find that the series conductance $g_s$ almost reaches a unitary limit value $2e^2/h$ only around cross-over regions of electron-configuration in double quantum dot. Next, we discuss the parallel conductance $g_p$ in three limit cases. From the similar discussion for two-terminal series configuration, we can easily understand the schematic pictures of electron-configuration in four-terminal parallel configuration for three limit case, shown in Fig. 2(b). For the case 1, our system is decoupled to two same systems composed of single-dot connected to two leads. In each system, one electron occupies single dot as shown in the picture [case 1] in Fig. 2(b), and causes Kondo effect. Therefore, the parallel conductance $g_p$ reaches a unitary limit value equal to $4e^2/h$ of two conducting modes. From Fig. 2(b), we indeed find that there is plateau of the parallel conductance $g_p$, which almost reaches a unitary limit value $4e^2/h$, for small values of $t/\Gamma$ and $U'/U$. The even-parity bonding orbital of double-dot is fully occupied by the two electrons in the case 2. In the case 3, two electrons fully occupy either of two dots and no electron occupies the other, as shown in the picture [case 3] in Fig. 2(b). Therefore, the parallel conductance in both case 2 and 3 is 0. This corresponds to the fact that the parallel conductance for large values of $t/\Gamma$ or $U'/U$ is suppressed to almost zero, as shown in Fig. 2(b). Fig. 2(a) is consistent with the phase diagram obtained by Mravlje et al. using Gunnarsson and Schönhammer projection-operator method 3, apart from details.

We consider also impurity entropy $S$ and impurity spin susceptibility $\chi$ calculated using NRG eigen-energy. In Fig. 3, we show the temperature dependence of (a) impurity entropy $S$ and (b) $\chi T$ for three points in $t/\Gamma - U'/U$ plane shown in Fig. 2(c): $(t/\Gamma, U'/U) = (0.0001, 0.2)$, $(t/\Gamma, U'/U) = (10, 0.2)$ and $(t/\Gamma, U'/U) = (0.0001, 1.5)$. For $(t/\Gamma, U'/U) = (0.0001, 0.2)$, impurity entropy shows steps of ln4 at $T/D \approx 10^{-4}$ and vanishes as temperature decreases. There is a corresponding shoulder in impurity susceptibility. It implies that the ln4 step originates from the degree of spin freedom. We can understand these thermodynamic behavior from consideration of the case 1. Each 1/2 - spin in single dot of two same systems for the case 1 is screened by Kondo effect in the same manner. Therefore total entropy $2xh2=ln4$ decays to 0 all at once. The impurity entropy and susceptibility for $(t/\Gamma, U'/U) = (10, 0.2)$ decrease and vanish at high-temperature $T/D \approx 10^{-3}$. This is because, in the case 2 assigned for $(t/\Gamma, U'/U) = (10, 0.2)$, the even-parity bonding orbital of double-dot stabilized by large hopping $t$ is fully occupied by the two electrons and the freedom of spin and orbital are quenched at $T/D \approx 10^{-3}$. For $(t/\Gamma, U'/U) = (0.0001, 1.5)$, a plateau of ln2 is seen in the impurity entropy as temperature decreases. The impurity spin susceptibility does not change around temperature region $10^{-13} \leq T/D \leq 10^{-11}$ where the impurity entropy begins to drop from ln2 to 0. Therefore, we find that the ln2 entropy is made up of the degree of orbital freedom. The ln2 plateau corresponds to non-Fermi liquid ground state with residual entropy in the case 3. But for $(t/\Gamma, U'/U) = (0.0001, 1.5)$, a finite $t$ results in Fermi liquid ground state and thereby the impurity entropy vanishes as temperature is lowered.

In summary, we have studied transport through a half-filled double quantum-dot with interdot repulsion in two-terminal series and four-terminal parallel configuration, the electron number in even-parity orbital, impurity entropy and spin susceptibility, using NRG method. Through the behavior of these quantities, we have presented the relation between transport and electron-configuration of double quantum dot in wide parameter region.

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Figure 2. (a) series conductance $g_s/(2e^2/h)$, (b) parallel conductance $g_p/(2e^2/h)$ and (c) electron number in even-parity orbital plotted as functions $t/\Gamma$ and $U'/U$. In (a) and (b), schematic picture of electron-configuration for case 1, case 2 and case 3 are presented.

Figure 3. The temperature dependence of (a) impurity entropy $S$ and (b) $\chi T$ for three points in $t/\Gamma - U'/U$ plane shown in Fig. 2(c); $(t/\Gamma, U'/U) = (0.0001, 0.2)$, $(t/\Gamma, U'/U) = (10, 0.2)$ and $(t/\Gamma, U'/U) = (0.0001, 1.5)$.

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