Ferromagnetically coupled magnetic impurities in a quantum point contact

Taegun Song and Kang-Hun Ahn
Department of Physics, Chungnam National University, Daejeon 305-764, Republic of Korea
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We investigate the ground and excited states of interacting electrons in a quantum point contact using exact diagonalization method. We find that strongly localized states in the point contact appear when a new conductance channel opens due to momentum mismatch. These localized states form magnetic impurity states which are stable in a finite regime of chemical potential and excitation energy. Interestingly, these magnetic impurities have ferromagnetic coupling, which shed light on the experimentally observed puzzling coexistence of Kondo correlation and spin filtering in a quantum point contact.

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Since two decades ago, it has been known that the conductance of a quantum point contact (QPC), a narrow constriction between two-dimensional electron gas, has plateaus at integer multiples of $2e^2/h$\cite{1}. This conductance quantization is due to the fact that the density of states of one-dimensional conductor is inversely proportional to the electron velocity, which is now well understood within Landauer formalism\cite{2}. Additional structure of the extra plateaus around $0.7(2e^2/h)$, has been observed, but the origin of the structure has been controversial ever since its observation\cite{3,4}. It has been suggested that the anomalous feature might be due to Kondo correlation because, similar to Kondo effect, there exist a zero-bias peak in the differential conductance which splits in a magnetic field and a crossover to perfect transmission below a characteristic temperature\cite{4}.

The Kondo interpretation as an origin of 0.7 structure, however, is questioned mainly by two reasons. First, the counter-intuitive existence of the impurity state on top of the potential barrier. Second, spin-filtering effect has been observed in a quantum point contact\cite{5,6}, which is hardly explainable within the Kondo model. The spin filtering effect is better explained by a phenomenological spin polarization model\cite{7} which assumes also counter-intuitive low-dimensional spontaneous spin polarization. In this Letter, we provide generalized view allowing both Kondo correlation and spin filtering by confirming the existence of the ferromagnetically coupled magnetic impurities in a quantum point contact. We will demonstrate the existence of the magnetic impurity in a QPC through exact diagonalization technique and show that the magnetic impurities are ferromagnetically coupled. Our numerical results imply that the transport through a QPC may have both Kondo correlation and spin-polarized transport due to the interplay between ferromagnetically coupled magnetic impurities.

Let us consider a quantum point contact modeled by a harmonic potential locally formed in a two dimensional electron system shown in Fig. 1 (a). The single particle Hamiltonian $h$ for this system is given by

\begin{equation}
\hat{h} = -\frac{\hbar^2}{2m^*} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + v(x, y) \tag{1}
\end{equation}

\begin{equation}
v(x, y) = \frac{1}{2} m^* \omega_0^2 y^2 \Theta\left(\frac{a}{2} - x\right) \Theta\left(x - \frac{a}{2}\right), \tag{2}
\end{equation}

where $m^*$ is the band effective mass of electron, $\omega_0$ is the natural angular frequency of the harmonic confinement of the point contact in transverse direction, and $\Theta(x)$ is the Heaviside step function. We impose periodic boundary condition for $x$ direction ($-L_x/2 < x < L_x/2$) and hard-wall boundary condition for $y$ direction ($-L_y/2 < y < L_y/2$). Here, $|x| < a/2$ is the regime of the quantum point contact and $a/2 < |x| < L_x/2$ describes the regime of the electron reservoir. By diagonalizing the Hamiltonian in Eq. (2) using eigen-wavefunction for $v = 0$ as

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{(a) Three dimensional plot of electric potential for a quantum point contact. (b) Probability density $|\psi(x)|^2$ of 206th eigen-state showing the first resonant level in QPC, and (c) the probability density of the 238th state showing the second resonant level. The parameters for the system size $L_x = L_y = 43.30 l_0$ and $a = 8.66 l_0$ where $l_0 = \sqrt{\frac{\hbar}{m^* \omega_0}}$.}
\end{figure}
basis wave functions, we obtain eigen-wavefunction $\psi_i(\mathbf{r})$ satisfying $\hbar \psi_i = \epsilon \psi_i$.

When a new transport channel opens near $\epsilon = (n + \frac{1}{2})\hbar \omega_0$, transport states which have the electron velocity $\frac{d\mathbf{r}}{dt} = \frac{k}{\hbar}$ contribute to the electric conductance. The conductance quantization is due to the fact that the density of the transport states, $\frac{1}{2\pi^2} \frac{dk}{d\epsilon}$, is proportional to the inverse of the velocity. This is Landauer formalism, where it is assumed that an electron out of the conductor does not scatter back to the conductor. The back-scattering, however, becomes significant when the momentum mismatch at the ends of the conductor is serious. In terms of the parameters for the QPC model in Eq. (2), we can write the momentum mismatch condition can be written as $\hbar \omega_0 \gg \frac{\pi^2 \hbar^2 l^2}{2m^* a^2}$. If this condition is met, the wavefunction at the ends of the point contact, $x = \pm \frac{a}{2}$, is close to zero due to the continuity of $\frac{\partial \psi}{\partial x}$.

The resonance condition for the existence of the standing wave in QPC, $ka = \pi, 2\pi, 3\pi, \cdots$, gives us good estimation of the electron energies showing the resonance;

$$\epsilon_{nl} \approx (n + \frac{1}{2})\hbar \omega_0 + \frac{\pi^2 \hbar^2 l^2}{2m^* a^2}, \quad (\hbar \omega_0 \gg \frac{\pi^2 \hbar^2 l^2}{m^* a^2})$$

(3)

where $n = 0, 1, 2, \cdots$ is the transport channel index and $l = 1, 2, 3, \cdots$ is the index for the resonant levels. Our numerical results confirm the estimation in Eq. (3) (not shown). Interestingly, low-level resonance shows strong enhancement of probability density $|\psi|^2$ in the QPC regime (See Fig. 1 (b) and (c) ). Note that, in contrast to the previous analysis[9], the localization here does not originate from electron interactions but from momentum mismatch. As will be shown later, due to the electron interaction, the localized states become singly occupied and thus magnetic impurities.

An Anderson magnetic impurity model has been introduced to account for the Kondo features of 0.7 anomaly[8]. Numerical calculations based on spin-density functional theory are suggestive of the existence of the magnetic impurity states[9, 10]. Since the density functional theories, however, are valid only for the ground state, it is questionable whether spin density functional theory can be applied to the Kondo effect where the magnetic impurity plays dynamical role. The exact diagonalization method can be used to investigate not only the ground state but also excited states of interacting electrons, thus it allow us to study whether the magnetic impurity can survive low energy excitation.

To obtain eigenstates of interacting electrons, we use a many-body Hamiltonian for electrons in the form:

$$H = \sum_{i,j} \epsilon_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} + \frac{1}{2} \sum_{i,j,k,l,\sigma,\sigma'} V_{ijkl} c_{i,\sigma}^\dagger c_{j,\sigma} c_{k,\sigma'} c_{l,\sigma'}$$

(4)

where $c_{i,\sigma}$ is annihilation operator for the i-th single particle eigenstate of h with spin $\sigma$, and

$$V_{ijkl} = \int d\mathbf{r} \int d\mathbf{r}' \psi_i^*(\mathbf{r}) \psi_j^*(\mathbf{r}') \frac{\epsilon^2}{|\mathbf{r} - \mathbf{r}'|} \psi_k(\mathbf{r}) \psi_l(\mathbf{r}')$$

(5)

We use Slater-determinant states for spin-up and spin-down electrons such as $| \circ \circ \circ \circ \cdots | \circ \circ \circ \cdots >$ for many-electron base vectors, where $\circ$ and $\bullet$ denote the occupied and unoccupied state, respectively. The circles in the left (right) of $|$ denote the spin up (down) states. We calculate many electron eigenstates up to 50 electrons where maximum matrix size is up to 11532 × 11532.

In Fig. 2 (a), we plot the net spin in units of $\hbar$ ($S_z = \frac{1}{2}(N_{up} - N_{down})$) of the ground state as a function of the total number of electrons $N = N_{up} + N_{down}$. In usual set-up of experiments, a gate voltage $V_g$ of quantum point contact is proportional to the chemical potential $\mu$. The total number of electrons $N$ is roughly proportional to the gate voltage since:

$$V_g \propto \mu = E_N - E_{N-1} \propto N,$$

(6)
where \( E_N \propto N^2 \) is the ground state energy of \( N \) interacting electrons. Thus, the gate voltage \( V_g \) dependence of the spin polarization can be probed by varying the number of electron \( N \) as in Fig.2 (a). The electron-electron interaction induces spin polarization of the electrons in the ground state in consistent with the density functional theory calculations. The spontaneous spin polarization is due to Hund coupling of electrons which are strongly bounded in the quantum point contact. Fig. 2 (a) and (b) show that the appearance of the spin-polarized regime (39 \( \leq N \leq 45 \) accompanies the single occupancy of the resonant levels. This is the regime where a transport channel begins to open as the gate voltage increases.

The single occupancy \(< n_i >= < n_{i\uparrow} > + < n_{i\downarrow} > \approx 1 \) is necessary condition for the magnetic impurity in the Kondo effect. This indeed happens as shown in Fig. 2 (b). As the total number of electron \( N \) (or the gate voltage ) increases, the first resonant level ( say \( r_1 \), of which probability density shown in the left inset) becomes singly occupied ( filled circle ). There exists a finite regime of \( N \) ( 39 \( \leq N \leq 42 \) and so the corresponding regime of \( V_g \) for \(< n_{r_1} > \approx 1 \). The first resonant level becomes no more magnetic impurity as it becomes doubly occupied for \( N \geq 43 \). Instead, the second resonant level, \( r_2 \), takes the role of magnetic impurity for \( N \geq 43 \) (empty diamonds). In the intermediate regime \( 40 \leq N \leq 42 \), both of the resonant levels \( r_1 \) and \( r_2 \) are singly occupied.

The polarized spins are distributed mainly near the center of quantum point contact as shown in Fig. 2 (c) and (d) where we plot the spin density \(< S_z (r) > \) for the ground states of \( N = 39 \) and \( N = 40 \):

\[
S_z (r) = \sum_{i,j} \psi_i^\dagger (r) \psi_j (r) [c_{i\uparrow}^\dagger c_{j\uparrow} - c_{i\downarrow}^\dagger c_{j\downarrow}]
\]  

(7)

Note that by adding one more electron to \( S_z = 1 \) state (Fig. 2 (c) ), the spin in the regime of quantum point contact is enhanced to be \( S_z = 2 \) (Fig. 2 (d) ) , i.e., the spins of singly occupied states are ferromagnetically coupled.

In Fig. 3, we plot the occupation numbers of two localized states \( r_1 \) and \( r_2 \) where their probability densities are shown in the left and right inset of Fig. 2 (b), respectively. If the magnetic impurity picture is valid for a quantum point contact at finite bias and temperatures, there must be low-lying many-electron excited states which have single occupancy in the localized state. This is indeed the case for the first resonant level \( r_1 \) so that \( < n_{r_1} > \approx 1 \) denoted by the horizontal solid arrow in Fig. 3 (a). However, the second resonant level is singly occupied \( < n_{r_2} > \approx 1 \) only in the ground state and it becomes almost empty even in the first excited state \( < n_{r_2} > \approx 0 \) as shown by the dotted arrow in Fig. 3 (b). This implies that the localization in the second resonant level is unstable against energy excitation. The electron in the second resonant level can easily escape out of QPC by applying a weak bias when the first resonant level is singly occupied, which could not be seen in the previous study based on density functional theory. When the gate voltage increases further, the second level again forms a stable magnetic impurity and the first level becomes doubly occupied ( not shown).

The observation mentioned above allows us to introduce an Anderson Hamiltonian for two resonant levels which describes low-lying excitations of the interacting electrons in QPC,

\[
H = \sum_{\sigma,i;1,2} \epsilon_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma} + \sum_{\sigma,k;L,R} \epsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma}
\]

\[
+ \sum_{i=1,2} U^{(1)} n_{i\uparrow} n_{i\downarrow} + \sum_{\sigma;i=1,2,k;L,R} [V^{(1)}_{k\sigma} c_{k\sigma}^\dagger d_{i\sigma} + H.c.]
\]

\[
- J_F \vec{S}_1 \cdot \vec{S}_2,
\]

(8)

where \( n_{i\sigma} = d_{i\sigma}^\dagger d_{i\sigma} \), \( \vec{S}_i = \sum_{\sigma',\sigma} d_{i\sigma'}^\dagger \sigma_{\sigma,\sigma'} d_{i\sigma'} \), \( \epsilon_{1\sigma} < \epsilon_{2\sigma} \) are on-site energies of the localized states, \( U^{(1)} > U^{(2)} \) are their on-site Coulomb energies, \( J_F \) is the ferromagnetic coupling strength between the localized states. \( V^{(1)}_{k\sigma} < V^{(2)}_{k\sigma} \) is the coupling strength between the localized state and the lead states created by \( d_{i\sigma}^\dagger \) and \( c_{k\sigma} \), respectively.

While the conductance calculation of the above model is not performed here, we sketch the possible transport mechanisms expected from the model in Eq.(8) ( See Fig. 4). When the chemical potential \( \mu \) approaches the value for a new channel opening, \( \epsilon_1 < \mu < \epsilon_2 - J_F \), the
first localized state becomes a magnetic impurity giving rise to the Kondo transport (see Fig. 4 (a)). If both of the localized states are singly occupied when \( \epsilon_2 - J_F < \mu < \epsilon_1 + U^{(1)} \), Kondo resonance through the first localized state will be hindered due to the ferromagnetic coupling with the second localized state. In this regime, spin-polarized transport is possible via enhanced g-factor through ferromagnetic coupling between the localized states. The spin polarized transport will be again weakened, if the first localized state becomes doubly occupied when \( \mu > \epsilon_1 + U^{(1)} \).

In the experiments showing spin filtering effects\,[3, 6], while an external magnetic field was applied, its strength was considered to be too small to polarize electron spin \((g\mu_B B < k_BT)\). The ferromagnetic coupling between the localized states, however, can strongly enhance the spin splitting. The ferromagnetic coupling can enhance the spin splitting of the second localized state \( \Delta \approx g\mu_B B + 2J_F (\langle n_{1\uparrow} \rangle - \langle n_{1\downarrow} \rangle) \approx g\mu_B B + 2J_F \tanh(\frac{g\mu_B B}{2k_BT}) \). Provided the ferromagnetic coupling \( J_F \) is large enough compared to the thermal energy, the spin splitting of the first localized state is given by \( \Delta \approx J_F g\mu_B B/k_BT \) \((J_F \gg k_BT \gg g\mu_B B)\).

The condition for the spin-polarized transport, \( \Delta > k_BT \), then becomes a experimentally reachable condition:

\[
\sqrt{J_F g\mu_B B} > k_BT. \tag{9}
\]

In the spin polarization measurement experiments\,[3, 6], typical electron interaction energy and the ferromagnetic coupling is about the order of \( J_F \approx 1 \text{meV} \), the bare Zeeman splitting is the order of \( g\mu_B B \approx 1 \mu\text{eV} \). Thus, the spin splitting in a quantum point contact is expected to be enhanced by two orders of magnitude: \( \sqrt{J_F g\mu_B B} \approx 100 \), which makes the effective spin splitting \( \Delta \) comparable to the thermal energy \( k_BT \). It is worth noting that similar models on the transport through double dot show spin-polarized transport\,[15, 19].

In summary, our numerical results based on exact diagonalization method show that localized states appear as resonant energy levels when a new conductance channel opens, and the magnetic impurities indeed exist as also excited states of interacting electrons. Thus, we confirm the Kondo magnetic impurity in a quantum point contact. Interestingly, the magnetic impurities have ferromagnetic coupling with each others which is expected to cause spin polarized transport. Our numerical calculation strongly supports that the counter-intuitive coexistence of Kondo correlation and spin filtering in a quantum point contact is due to ferromagnetically coupled magnetic impurities in the quantum point contact. The existence of the magnetic impurity in our work is in consistent with the recent experimental evidence for the bound state in quantum point contact probed with coupled QPCs\,[20].

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