Ferromagnetic Spin Coupling as the Origin of 0.7 Anomaly in Quantum Point Contacts

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We study one-dimensional itinerant electron models with ferromagnetic coupling to investigate the origin of 0.7 anomaly in quantum point contacts. Linear conductance calculations from the quantum Monte Carlo technique for spin interactions of different spatial range suggest that 0.7(2e^2/h) anomaly results from a strong interaction of low-density conduction electrons to ferromagnetic fluctuations formed across the potential barrier. The conductance plateau appears due to the strong incoherent scattering at high temperature when the electron traversal time matches the time scale of dynamic ferromagnetic excitations.

Quantum point contacts (QPC) are narrow constrictions inside two-dimensional electron gas. They construct one of the building blocks of submicrometer devices such as quantum dots and qubits. The dc conductance through a QPC is quantized in steps of G_0 = 2e^2/h. However, experiments also reveal the appearance of an additional shoulder in the conductance measurement near 0.7G_0 widely referred to as the 0.7 anomaly. The origin of 0.7 anomaly in QPC has remained a puzzle over almost a decade. The evolution of the 0.7G_0 plateau to 0.5G_0 with magnetic field and the enhancement of the g factor have strongly suggested that the origin of the anomaly is the electron spin.

A number of scenarios have been proposed, such as spin polarization of the itinerant electrons, ferromagnetic correlation, formation of a spin 1/2 magnetic moment in the conductance channel, and Kondo effect. Hubbard chain, Wigner crystallization and antiferromagnetism. These approaches have produced a wide range of different phenomenologies, sometimes inconsistent with experiments, and there is no widely accepted microscopic theory to date. The problem is partly due to the approximate methods used in the strongly interacting limit and therefore it becomes essential to perform exact calculations to test microscopic models against experiments. Here we use numerically accurate quantum Monte Carlo technique to study the strong correlation effects in QPC devices.

We find that the 0.7 anomaly at high temperature arises from the incoherent electron scattering from itinerant ferromagnetic fluctuations near the Stoner instability in the strong correlation limit of low electron density created by spatially inhomogeneous gate potential. We show, through a comparison with a model with on-site interactions, that the relevant electron scattering is due to the spin fluctuations which are spatially coherent across the potential barrier. With decreasing temperature, the magnetic excitation becomes slower than the itinerant electrons. The current is then carried by the quasiparticles and the 0.7 plateau gradually disappears. With the Zeeman magnetic field, the 0.7 plateau evolves to a robust 0.5 plateau in agreement with experiments.

We model our system using a one-dimensional (1D) electron gas with spin-spin interaction among itinerant electrons as depicted in the figure. The gate voltage potential V(x) acts as an adiabatic potential barrier through the QPC region. A bias with a ramp passing through the QPC is applied across the chain to compute the dc conductance in the linear response regime.

The Hamiltonian reads

\[ H = \int dx \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) - \mu + \frac{1}{2} \bar{\sigma} \cdot \vec{H} \right\} \psi(x) + \int dx \left\{ K_1(x) [\bar{s}(x)]^2 + \frac{1}{2} K_2(x) [\partial_x \bar{s}(x)]^2 \right\} \]

with \( \psi(x) = [\psi_1(x), \psi_2(x)]^T \) the field operator vector, \( \mu \) the chemical potential, \( H \) the Zeeman magnetic field, \( \bar{\sigma} \) the Pauli matrices and \( V(x) \) the external gate voltage barrier in order to pinch off the electron current through the QPC. \( V(x) \) is defined in our model as \( V(x) = V_g / \cosh(s(x)/L_g) \) with \( x = 0 \) corresponding to the center of the chain, \( L_g \) a characteristic length and \( V_g \) the gate voltage. The operator \( \bar{s}(x) = \psi^\dagger(x) \frac{\partial}{\partial x} \psi(x) \) represents the spin density of itinerant electrons along the chain. Spins interact locally with the coupling constant \( K_1(x) = \alpha(x) K_1 \) \( (K_1 < 0 \) for repulsive on-site Coulomb interaction) with \( \alpha(x) = 1 / \cosh(s(x)/L_s) \) an attenuating function with characteristic length \( L_s \). We set the spin coupling to adiabatically fall off to take into account the screening effects in the leads and to reduce the backscattering due to interaction away from the QPC.
constriction. $K_2(x) = \alpha(x) K_2$ ($K_2 > 0$) is the coefficient of the gradient term accounting for the ferromagnetic Heisenberg interaction. We discretize the continuum model Hamiltonian to a tight-binding chain of lattice constant $\Delta x$ with the nearest-neighbor hopping $t$. Defining $t = \frac{\hbar^2}{2m_{leff} \Delta x}$, $\mu = \mu - \frac{\hbar^2}{2m_{leff} \Delta x} \sqrt{\Delta x} \psi(x_i) = c_i$, $J_0 = -\frac{\hbar^2}{\Delta x^2} + \frac{\hbar^2}{\Delta x^2}$, $J_1 = \frac{\hbar^2}{\Delta x^2}$ and $\vec{s}_p = c_p^\dagger \vec{e} c_p$ the discretized Hamiltonian reads

$$
\mathcal{H} = -t \sum_{<ij>,\sigma} c_i^\dagger c_j^\sigma - \sum_{\sigma} \left( \mu - V_i + \frac{1}{2} \sigma H \right) c_i^\dagger c_i^\sigma
$$

$$
- \sum_{p \in \text{block}} \left( J_0 \alpha_p^2 \vec{s}_p \cdot \vec{s}_p + J_1 \alpha_p \alpha_{p+1} \vec{s}_p \cdot \vec{s}_{p+1} \right),
\tag{2}
$$

with $H$ taken along the $z$ direction and $\sigma = \pm 1$ the spin index. The microscopic parameters $K_1$ and $K_2$ are unknown and we treat $J_0, J_1 > 0$ (for ferromagnetic coupling) as the model parameters throughout this letter. The index $p$ runs only within the interacting block in Fig.1 near the QPC saddle point. The discretization is valid since we are in the low-density limit with $\langle c_i^\dagger c_i \rangle < 1$ inside the interacting block. Near the pinch-off gate voltage, $\langle c_i^\dagger c_i \rangle$ at the top of the potential barrier rapidly approached zero in the following calculations. Using $m = 0.067 m_e$ for GaAs and $\Delta x \approx 20$ nm (experimental QPC length is around 200 nm, roughly $10 \Delta x$ for $L_g = 4$), $t = 1.4$ meV. Due to CPU limitations, we restrict the interacting block to about seven sites.

In our calculations, we modify Eq.(2) by allowing the nonlocal part of the interaction term to extend beyond nearest neighboring sites. We define the block spin operator $\vec{S} = \sum_{p \in \text{block}} \alpha_p \vec{s}_p$, and rewrite a new Hamiltonian

$$
\mathcal{H} = -t \sum_{<ij>,\sigma} c_i^\dagger c_j^\sigma - \sum_{\sigma} \left( \mu - V_i + \frac{1}{2} \sigma H \right) c_i^\dagger c_i^\sigma
$$

$$
- \sum_{p \in \text{block}} \left( J_0 - \frac{J_1}{2} \right) \alpha_p^2 \vec{s}_p \cdot \vec{s}_p - \frac{J_1}{2} \vec{S} \cdot \vec{S},
\tag{3}
$$

Compared to Eq.(2), Eq.(3) incorporates stronger spin interaction among all the spins within the interacting block. This modification makes the decoupling scheme in quantum Monte Carlo more efficient. Interactions beyond nearest neighbors can be thought of a coarse-grained effective Hamiltonian on the discretized lattice in the low wave-vector limit. The effective interaction results from virtual fluctuations to high momentum states which are excluded in the discretized model and it takes a form similar to the RKKY interaction. Since we are interested in the low-density limit near the pinch-off regime with the effective Fermi wave-vector $k_{F,eff}$ inside the constriction approaching zero, the $k_{F,eff} R_i$ factor for position $R_i$ inside the constriction also goes to zero and the effective spin interaction over the interacting block becomes predominantly ferromagnetic.

We use a continuous Hubbard-Stratonovich decoupling for the $\vec{S} \cdot \vec{S}$ term in Eq.(3) and discrete decoupling for local $\vec{s}_m \cdot \vec{s}_m$ term. We calculate the dc conductance using the Kubo formula in the linear response regime, $G_{dc}(\omega = 0) = \lim_{\nu \to 0} \text{Re} \int_{-\infty}^{\infty} e^{i\omega t'} \langle [j(t'), H_{sd}] \rangle dt'$, where $j(t') = i \eta \sum_{\sigma} [c_i^\dagger (t') c_i \sigma (t') - c_i^\dagger \sigma (t') c_i (t')]$ is the current operator evaluated at the center of the QPC and $H_{sd} = -e \sum_{m,s} V(x_m) n_{m,s}$ is the external perturbation across the chain with $V(x_m)$ the normalized source-drain bias with maximum (minimum) voltage $1/2 (-1/2)$ on the (left) (right) side as depicted in Fig.1. The range of summation in $H_{sd}$, $|m| \leq 100$, produced well-converged conductance. Conductance by the Kubo formula is obtained in terms of the bosonic Matsubara frequencies ($\nu_n = \frac{\pi n}{2 T}$ where $\beta = 1/k_B T$ with $k_B$ the Boltzmann constant and positive integer $n$) and it needs to be analytically continued to real frequency to take the dc limit $G_{dc}(\omega = 0)$. This task is done by fitting the conductance defined on the Matsubara frequency into the Lehman representation $G(i\nu_n) = i \int_{-\infty}^{\infty} dw \rho'(w)\frac{\rho(w)}{\nu_n - w}$ with the spectral function $\rho'(w)$ as the fitting parameter. This method has been extensively tested to an excellent agreement in comparison with the rational function fit [29]. After taking the analytic continuation $i\nu_n \to \omega + i\eta$, we obtain the conductance $G_{dc}(\omega = 0) = \rho(0)$.

Fig.2(a) plots the dc conductance as a function of the gate voltage $V_g$ at different values of $L_g$ and $L_s$ at several $J_0$ and $J_1$ values and fixed chemical poten-
the gate potential at zero field, it is inconsistent with the 0.7 phenomenological feature for $T = 0.014t$.

We must also capture the correct trend as seen in the experiment. Despite the phase problem of the quantum magnetic field is applied. The significantly wide splitting ($\Delta V_g = 0$), falling within the experimental range [16].

Fig. 2(b) exhibits the gradual evolution of the plateau near $0.15$. Fig. 2(c) shows that, with decreasing temperature, the conductance plateau consistently moves upward with decreasing width. Despite the phase problem of the quantum Monte Carlo method for temperature $T < 0.014t$, we are able to capture the correct trend as seen in the experiment for $0.014t \leq T \leq 0.033t$. $T = 0.025t$ corresponds to $T \approx 0.41K$, falling within the experimental range [16].

Features in Fig. 2(a)-(c) correctly reproduce the experimental results on the temperature and magnetic field dependence.

Fig. 2(d) plots the conductance in the purely local limit ($J_1 = 0$). The local spin model is equivalent to the repulsive Hubbard model [20, 21, 22, 23] with the on-site Coulomb parameter $U$ given as $U = 3J_0/4$ by redefining the gate potential $V_g$ to absorb the one-body terms. Although the local limit produces a well-defined 0.7 feature at zero field, it is inconsistent with the 0.7 phenomenology. First, the 0.7 feature becomes more pronounced as temperature is lowered. Second, more interestingly, at finite magnetic field two plateaus appear with the 0.7 feature shifted to higher conductance and another plateau emerging near $G \sim 0.3G_0$. It is very interesting that these results are consistent with the scenario of spin singlet-triplet formation discussed in Refs. [18, 20]. The main difference here is that the spin is self-generated from itinerant electrons in our model, not as an external spin [18] or from a quasibound state [20]. Near the pinch-off, electron and spin densities are low and the spin-singlet does not form and the conductance plateau does not appear at $H = 0$. However, at finite $H$, the spin moment becomes enhanced enough to produce the spin-singlet conductance plateau.

In the presence of nonlocal interactions, an itinerant electron interacts with many neighboring sites and the resulting spin multiplets are not necessarily $S = 0$ or $S = 1$. With the finite interacting range, a spatially coherent ferromagnetic state extends over the interacting block at finite $H$ and becomes harder to be flipped by electron scattering. Therefore, the nonlocal interaction blocks the minority-spin band and the 0.5 plateau results from spin splitting, instead of the 0.3 plateau through the singlet formation. It has been shown previously that ferromagnetic coupling beyond local interaction stabilizes the ferromagnetic phase in a uniform 1D chain [14].

Due to the low electron density within the constriction at the pinch-off, the ferromagnetic spin correlations are considerably enhanced at low $T$. We compute the ferromagnetic spin correlation function (FSCF), $C_{FM}(n) = \frac{1}{N} \sum_{p,m} \langle \tau \rangle \langle S_p^+ \rangle \langle S_m^- \rangle$, with $\langle \tau \rangle = \frac{\tau}{\pi} (n \geq 0)$ the bosonic Matsubara frequency, $\tau$ the imaginary time and $N$ the number of sites inside the interacting block in Fig. 1. Fig. 3(a) plots the static FSCF ($\nu_{\omega} = 0$) as a function of $V_g$ at different $T$ values corresponding to the conductance curves in Fig. 2(c). In comparison, the gate potential at zero field, it is inconsistent with the 0.7 phenomenological feature for $T = 0.014t$.
comparision with the noninteracting system, the static FSCF is significantly enhanced as $T$ is lowered when there is interaction. Enhancement of the static FSCF is effective only around the pinch-off due to the singular nature of the 1D density of states. The gate voltage range for the maximum enhancement of static FSCF also coincides with that of the plateaus in Fig. 2(a)-(c), indicating the effect of strong ferromagnetic correlations on the appearance of the plateau. The dynamic ferromagnetic spin susceptibility can be obtained by analytically continuing the FSCF using the same method employed for the conductance. Through the fluctuation-dissipation theorem, $\rho_{FM}(\omega)$, the spectral function for magnetic excitations can be obtained from the analytically continued $C_{FM}^{(+)}(i\nu_n \rightarrow \omega + i\eta)$ from positive $\nu_n$. In Fig. 3(b), $\rho_{FM}(\omega)$ has been plotted for different values of $V_g$ at $T = 0.025t$ corresponding to Fig. 3(a). The height of the peak grows as $V_g$ increases towards the pinch off, reaching its maximum for $V_g \approx 0.4t - 0.5t$, around $\omega_{peak} \approx 0.1135t$ as indicated by the dashed line. As $V_g$ is further increased, the height of the peak decreases in agreement to the decrease in the static FSCF in Fig. 3(a). However, the location of the peak continues to stay at $\omega_{peak} \approx 0.1135t$ as the characteristic excitation energy at $T = 0.025$ up to $V_g \approx 0.7t$ where ferromagnetic correlations have almost been obliterated as shown in Fig. 3(a).

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