Mean-Field Calculations of Transport Properties through Point Contact of Magnetic Metals

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The electric conduction through atomic-size point contacts of metals has attracted much attention these days. The conductance quantization in units of $2e^2/h$ has been observed in break-junctions of non-magnetic metals. For magnetic metals, Ono *et al.* have found that the conductance is quantized in units of $2e^2/h$ under magnetic fields smaller than 67 Oe, whereas the conductance is quantized in units of e^2/h under larger magnetic fields [1]. In the latter case, the spin polarization is expected to be in the same direction in the whole system (parallel alignment). In the former case, the magnetic domain wall should be formed around the point contact: The spin polarization on one side of the contact is anti-parallel to that on the other side (anti-parallel alignment).

We theoretically study the spin-dependent transport through point contacts of magnetic metals. The atomic structure around the contact is taken into account by tight-binding models (three-dimensional simple cubic lattice, for simplicity). The conductance in spin-polarized states is calculated, using a Green's function method to take into account the electron-electron interaction. We examine a single band model and two-band model [2], paying attention to the coexistence of broad s band and narrow d bands at the Fermi level, $E_{\rm F}$, in the transition metals.

In a single band model, an s orbital exists at each site. The Hamiltonian reads

$$\mathcal{H} = \sum_{i,\sigma} \epsilon_{\rm s} c_{i\sigma}^{\dagger} c_{i\sigma} + \sum_{\{i,j\},\sigma} (-t_{\rm s} c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow},$$

where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) creates (annihilates) an electron with spin σ at atom i. $-t_{\rm s}$ is the transfer integral between the neighboring atoms, $\{i,j\}$. The short-range Coulomb interaction U is taken into account by the Unrestricted Hartree-Fock (UHF) method. The spin-polarized state appears when U is larger than a critical value (Stoner magnetization of itinerant electrons). The conductance through a point contact (*e.g.*, geometry in Fig. 1) is obtained by the UHF self-consistent calculations using the Green's function. This is an extension of the Green's function method for non-interacting electrons [3]. We examine spin-polarized states (parallel alignment) in several geometries of the point contact and find that the conductance is quantized in units of e^2/h per spin.

In a two-band model, each site has two s-like orbitals, one (s orbital) forms a wide band and the other (s' orbital) forms a narrow band. The on-site Coulomb interaction U is assumed to exist only in the s' orbital. With U larger than a critical value, the spin-polarized state is realized (extended Stoner magnetization). We calculate the conductance in the geometry in Fig. 1, in the parallel and anti-parallel alignments of the spin polarization.

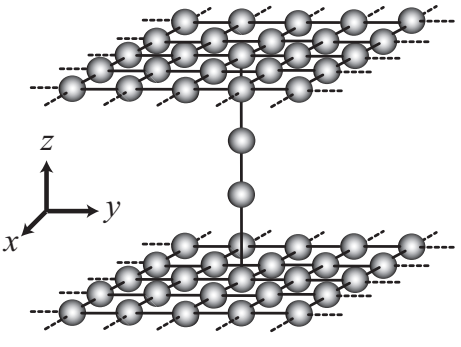

Fig. 1: A geometry of our tight-binding models. Two leads are semi-infinitely long in z direction and eight atoms wide with periodic boundary condition in both x and y directions. A sphere represents an atom which has single s orbital (single band model) or two s-like orbitals (two-band model). Electrons are transported between neighboring atoms connected by solid lines.

In Fig. 2(a), we show the conductance in the parallel alignment, as a function of the Fermi level $E_{\rm F}$. The total conductance G (curve a) is the sum of the conductance of spin-up electrons (curve b) and that of spin-down electrons (curve c). The total conductance shows a plateau of $G = 2.2e^2/h$, which consists of $G = 0.7e^2/h$ by spin-up electrons and $G = 1.5e^2/h$ by spin-down electrons. For spin-up electrons, the s' band is almost fully occupied while the s band is nearly half-filled around $E_{\rm F} = 0$ (see the inset in Fig. 2(a)). The number of conduction channels is unity since the former does not contribute the conductance. For spin-down electrons, the number of conduction channels is two because both s and s' bands are partly filled. If the conductance were quantized, the conductance would be e^2/h and $2e^2/h$ for spin-up and -down electrons, respectively. The above-mentioned values indicate the suppression of the conductance by 25%, which is in contrast to the case of single band. This is because the hybridization between s and s' orbitals differs between in the contact region and in the leads, which disturbs smooth transport of electrons through the point contact.

Figure 2(b) presents the conductance in the anti-parallel alignment of the spin polarization. In this alignment, the conductance of spin-up electrons is equivalent to that of spin-down electrons (curves b and c). The number of conduction channels is unity for each spin direction since the s' band is fulfilled in one of the leads (inset in Fig. 2(b)). The total conductance shows a plateau of $G = 2e^2/h$ (curve a). Hence the interband scattering is not relevant and the conductance is quantized in units of $2e^2/h$ in the anti-parallel alignment. This is in agreement with the experimental results [1] although our two-band model is simple.

[1] T. Ono *et al.*, Appl. Phys. Lett. **75**, 1622 (1999). [2] In our previous work for non-interacting electrons, the conductance is quantized in a single band model, whereas the conductance is significantly suppressed by the interband scattering in a two-band model [K. Ueno *et al.*, J. Phys. Soc. Jpn. **71**, 860 (2002)]. [3] T. N. Todorov *et al.*, J. Phys. Condens. Matter **5**, 2389 (1993).

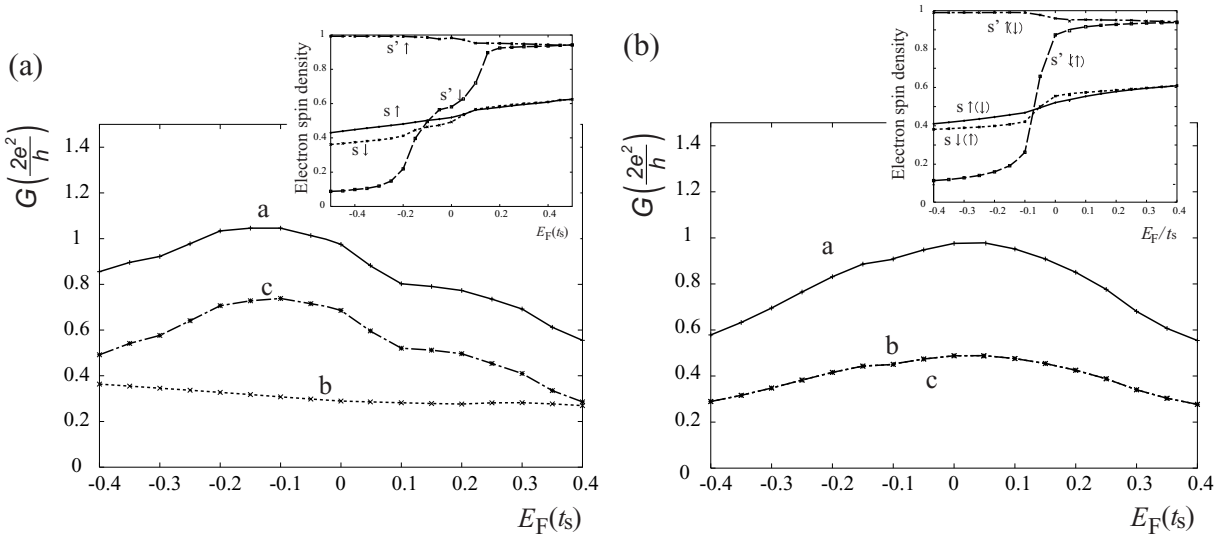

Fig. 2: The conductance through a point contact shown in Fig. 1 (two-band model), as a function of the Fermi level $E_{\rm F}$. The spin polarization is (a) in parallel alignment and (b) in anti-parallel alignment. The on-site energies of s and s' orbitals are $\epsilon_{\rm s} = 0$ and $\epsilon_{s'}/t_{\rm s} = -5$. The on-site repulsion is $U/t_{\rm s}$=5. Curve a represents the total conductance, which is the sum of the conductance of spin-up electrons (curve b) and that of spin-down electrons (curve c). Note that curves b and c are completely overlapped in (b). The transfer integral between s' (s and s') orbitals is $t_{s'}/t_{\rm s} = 0.1$ ($t_{{\rm s},s'}/t_{\rm s} = 0.5$). Inset: Electron spin density in each orbital at an atom of the point contact, as a function of $E_{\rm F}$.