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F-3-4 The effect of side-traps on ballistic transistor in Kondo regime

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1. Introduction

As the size of a Si-MOSFET (Metal-Field-Effect Field Effect Transistor) decreases, electronic transport of carriers is expected to change from the diffusive region to the ballistic region[1]. In this era, the gate insulator SiO_2 is replaced by higher dielectric constant materials (high-k materials), in which trap states cannot be avoided. Trap sites degrade device performance such as flat band voltage shifts. However, their effect on ballistic transport has not yet been clarified. On the other hand, the effect of side-trap states on infinite quantum wire (QW) is treated as Fano-Kondo (FK) problem and has attracted great interest where conductance is suppressed as a result of a destructive interference at $T < T_K$ (Kondo temperature) [2-4]. The infinite QW without the source and drain is not the situation of the future ballistic transistors. Here, we investigate the effect of trap site on ballistic transistor by Keldysh Green's function method based on slave-boson mean field theory (SBMFT)[5,6].

2. Formulation

We model the ballistic transistor as shown in Fig. 1 where two potential barriers exist between the electrodes (source and drain) and the ballistically conducting channel. The tunneling rates are written as Γ_L and Γ_R. This model can also be used for the Schottky transistors[7]. In the SBMFT, an infinite on-site Coulomb interaction for each trap site is assumed, which means that at most one excess electron is permitted in the trap site[5,6].

One trap site – First we consider the effect of one trap site (Fig.1(a)). The Hamiltonian is written in terms of slave-boson mean fields as $H = H_{\rm chan}^{(\rm I)} + H_{\rm elec} + H_{\rm tran}$. $H_{\rm chan}^{(\rm I)}$ represents the conducting channel and trap site:

$$H_{\rm chan}^{(\rm I)} = \sum_k \sum_{s=\uparrow,\downarrow} E_k c_{ks}^\dagger c_{ks} + \epsilon_f d_s^\dagger d_s + \sqrt{z}\sum_k \sum_{s=\uparrow,\downarrow} [V_d d_s^\dagger c_{ks} + {\rm h.c}] + (\epsilon_f - E_D)(z-1) \quad (1)$$

$H_{\rm elec}$ represents the two electrodes written as $H_{\rm elec} = \sum_{\alpha=L,R}\sum_{ks} E_{k\alpha} f_{ks}^{\alpha\dagger} f_{ks}^\alpha$, and $H_{\rm tran}$ describes transference of electrons between different regions, given by $H_{\rm tran} = \sum_{\alpha=L,R}\sum_{k_1k_2s}(t_{k_1k_2}^\alpha c_{k_1s}^\dagger f_{k_2s}^\alpha + {\rm h.c.})$. $f_{ks}^\alpha (\alpha = L,R)$, c_{ks} and d_s are, respectively, the annihilation electron operator for both electrodes, the channel region and the trap site. $E_{k\alpha}$ and E_D are the energies for the electrodes and trap site, respectively. ϵ_f is a quasiparticle trap energy. z is a mean value of the boson operator, showing the average vacancy rate in the trap site. ϵ_f and z are determined by self-consistent equations shown below. $t_{k_1k_2}^\alpha$ and V_d are the tunneling matrix between the channel region and the electrodes and that of conducting region and the trap site, respectively. This approximation is valid below $T_K \approx D\exp(E_D D/(2V_d^2\pi))$ (D is a band width) [5].

The current I_D between the source and drain is described by Keldysh Green's function as $I_D = (2e/h)\sum_{kk'}\int d\omega {\rm Re}\{t_{kk'}^L G_{c_{k'}f_k^L}^<(\omega)\}$ where $G_{c_{k'}f_k^L}^<(t,t') \equiv i\langle f_k^{L\dagger}(t')c_{k'}(t)\rangle$ [8](we neglect spin dependence). By using a relation $G^< = g_1^r g_2^< + g_1^< g_2^a$ when $G = g_1 g_2$, we can describe $G_{c_{k'}f_k^L}^<(t,t')$ by elementary Green's functions. First, the current without trap is derived as $I_0 = g_0 V_D$ (V_D is a drain voltage) where $g_0 = \frac{e}{h}\frac{y_0}{(1+y_0)^2}\frac{\Gamma_L\Gamma_R}{\gamma}$. $y_0 \equiv \pi N_c(E_F)\gamma$ is a number of channel electrons in the energy width of γ ($\gamma = (\Gamma_L+\Gamma_R)/2$ and $N_c(E_F)$ is a density of states in the channel region at Fermi energy E_F). Note that the energy dispersion E_k in the channel region has continuum k dependence. This is in contrast with that of a quantum dot discussed in Ref.[8,9] where band mixing of discrete energy-levels in the quantum dot can be neglected. I_D with a trap site is given as

$$I_D = g_0\int_{-D}^{D} d\omega \frac{(\omega-\epsilon_f)^2}{(\omega-\epsilon_f)^2 + z^2\eta^2}(f_L(\omega) - f_R(\omega)) \quad (2)$$

where $\eta = \eta_0 y_0/(1+y_0)$ with $\eta_0 = V_d^2/\gamma$. $f_L(\omega) \equiv (\exp((\omega - E_F + eV_D)/T) + 1)^{-1}$ and $f_R(\omega) \equiv (\exp((\omega - E_F)/T) + 1)^{-1}$ are Fermi distribution functions of the left and right electrodes (Boltzmann's constant $k_B = 1$). This formula is the main result of this paper and shows that the existence of trap site decreases I_D greatly when the energy of carrier electrons is close to the trap site energy. Compared with the infinite wire case[2,3], we can see that the coupling strength η is modified by y_0 and is a function of Γ_L and Γ_R.

The self-consistent equations for ϵ_f and z are given as

$$2\int_{-D}^{D}\frac{d\omega}{\pi}\frac{\eta(\omega-\epsilon_f)}{(\omega-\epsilon_f)^2+z^2\eta^2}F_1(\omega) = E_D - \epsilon_f \quad (3)$$

$$2\int_{-D}^{D}\frac{d\omega}{\pi}\frac{z\eta}{(\omega-\epsilon_f)^2+z^2\eta^2}F_1(\omega) = 1 - z \quad (4)$$

where $F_1(\omega) \equiv \{y_0[\Gamma_L f_L(\omega) + \Gamma_R f_R(\omega))]/(\Gamma_L+\Gamma_R) + f_c(\omega)\}/(1+y_0)$ and $f_c(\omega) \equiv (\exp((\omega - E_F + eV_D/2)/T) + 1)^{-1}$. In the $\gamma \to 0$ limit, these equations reduce to those given in Ref.[5]. As shown below, the V_D dependence of ϵ_f and z is week. In such case, we can analytically express conductance $G = dI_D/dV_D$ at $V_D = 0$ and $T = 0$:

$$G = g_0\frac{(E_F-\epsilon_f)^2}{(E_F-\epsilon_f)^2 + z^2\eta^2} \quad (5)$$

This formula says that G has a dip structure when ϵ_f coincides with E_F.

Two trap sites – As discussed in Ref.[5,6], the Hamiltonian of the channel part with two traps, $H^{(\mathrm{II})}_{\mathrm{chan}}$, is described as the summation of two independent parts consisting of symmetric ($P = +$) and antisymmetric($P = -$) parts, if there is no interaction between the two traps. Correspondingly, Hamiltonian with electrodes is described by the two independent parts. Then I_D and G consist of two independent parts. In particular G at $T = 0$ is

$$G = g_0 \sum_{P=\pm} \frac{(\epsilon_f - E_F)^2}{(\epsilon_f - E_F)^2 + z^2\eta_P^2} \qquad (6)$$

where $\eta_P = \eta_{P0} y_0/(1 + y_0)$ with $\eta_{P0} = (N_P V_d)^2/\gamma$ and $N_P \equiv (1+P\sin(k_F R)/k_F R)/2$ (R is the distance between the two traps). Thus, the dip in G is intrinsic and can be described in a similar fashion to the single trap case.

3. Numerical calculations

Figure 2 shows the conductance dI_D/dV_D at $V_D = 0.01\gamma$ when coupling constant η_0 is changed. We can see a deep dip structure near E_F. This is the result of the interference between the channel electrons and the trap site (FK effect). Figures 2 (a) and (b) also show that the result is irrelevant to the value of y_0. Here, the minimum T_K is larger than $T = 0.01\gamma$. Figure 3 shows, when the dip appears, the trap site is occupied by an electron ($z \sim 0$) and trap site energy ϵ_f increases. Figure 4 shows I_D-V_D curve at $E_D = -1.2\gamma$ where the dip appears. We can see that, as η_0 increases, I_D decreases rapidly. This indicates that the existence of trap site reduces the drive current. In Fig.5, we calculate G from Eq.(5) using ϵ_f and z in Fig.3. We found that the analytical formula Eq.(5) approximately reproduces the numerically differentiated results of Fig.2 (a).

Let us consider a simple estimation. The numerical calculations show that the clear dip can be seen when $\eta_0 \sim \gamma$. If we take $D \sim (\hbar^2/2m)(3\pi^2 n)$ with effective mass $m = 0.2m_0$ (m_0 is a free electron mass) and the channel electron density $n = 10^{-17}\mathrm{cm}^{-3}$, then $D \sim 4$meV. When γ is estimated from $I_D \sim e\gamma$ and $I = 0.1\mu$A, $\hbar\gamma \sim 0.4$meV. Then a broad dip structure would be observed at room temperature for the traps whose coupling energy is 0.4 meV.

4. Conclusion

We studied the effect of trap sites on transport of ballistic transistor and showed that conductance has an intrinsic dip as a result of the interference effect. This is an interesting interplay between physics and engineering devices.

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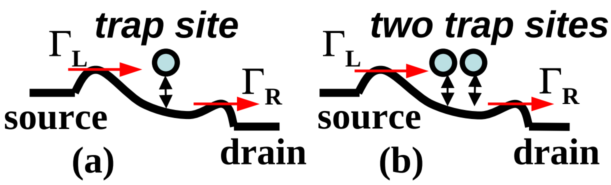

Fig. 1: Side-trap states near the conducting channel. (a) One trap site case. (b) Two trap sites case. Channel electrons can be trapped by these sites. Potential barriers are assumed to exist between the electrodes and the channel region.

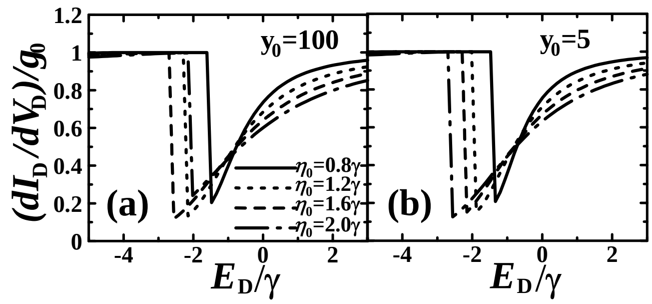

Fig. 2: Conductance dI_D/dV_D for a trap site (Fig.1 (a)) as a function of trap site energy E_D at V_D=0.01γ. (a) y_0=100. (b) y_0=5. D=6γ, E_F=0 and T=0.01γ. In this paper, we set Γ_L=Γ_R, and take γ=(Γ_L+Γ_R)/2 as an energy unit.

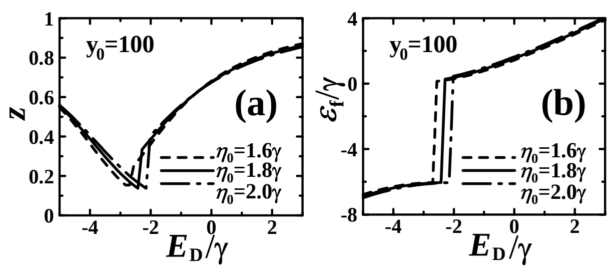

Fig. 3: Solutions for the self-consistent equations Eq.(3) and Eq.(4) as a function of E_D. (a) z and (b) ϵ_f. Parameters are the same as those in Fig.2. As z becomes closer to 0, the trap site is occupied with higher probability.

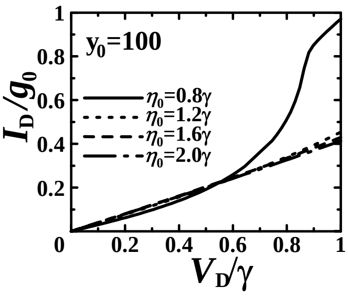

Fig. 4: I_D-V_D for a trap site (Fig.1 (a)). E_D =-1.2γ, y_0=100, D=6γ, E_F=0 and T=0.01γ.

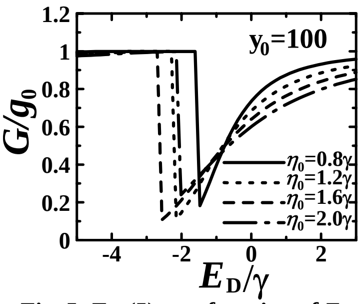

Fig. 5: Eq.(5) as a function of E_D, where self-consistent z and ϵ_f are used. Compared with Fig.2, we found that Eq.(5) is effective.