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Effect of Impurities on Tunnel Conductance in Finite Voltage and Temperature

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Transport phenomena through a tunnel junction in the presence of impurities in the insulating layer are investigated in the finite temperature and finite bias voltage. We have found that the effect of the temperature on the tunnel conductance in the non-linear current-voltage $(I-V)$ characteristics is smaller than that in the linear-response case.

Key words: transport phenomena, tunnel junction, non-linear response, impurity effect

1. Introduction

Spin-polarized transport phenomena in ferromagnetic metal(FM)/insulator/FM tunnel junctions have attracted current interest. The spin-polarized tunneling studies have been performed in order to access information about spin-dependent electronic states. In recent years, the transport phenomena in such systems are studied extensively, and large magnetoresistance ratio as much as 30 % has been reported in $Fe/Al_2O_3/Fe$[1] and $CoFe/Al_2O_3/Co$.[2] Although a great progress has been made in the experimental study, there remain some unsolved problems about tunnel conductance and tunnel magnetoresistance (TMR), *e. g.*, 1) thickness and barrier height of insulating layer dependence, 2) sample dependence, 3) temperature dependence, and 4) bias dependence. These problems are more or less related to the randomness in each layer.[3–5] Several theoretical works, such as Julliere[6] and Maekawa and Gäfvert,[7] associated with experiments on TMR have been done. The study of Maekawa and Gäfvert has assumed incoherent tunneling, in which the randomness could be included implicitly, however, it is not able to show how the randomness affects the TMR. Recently, Itoh *et al.* proposed a microscopic method which can treat the randomness explicitly to clarify the effect of the randomness on the tunnel conductance and TMR in the linear response regime.[8] They have performed numerical simulations for finite size clusters with the randomness and calculated the tunnel conductance and TMR. They showed that the direct calculation of the tunnel conductance is sufficiently effective.

In this study, we have used a microscopic model which can be applicable to the complex structure of the sample geometry *under finite bias voltages*. We constracted the model by extending that proposed by Itoh *et al.*[8] In spite of the importance of studying transports *under the finite bias voltages*, theoretical approaches seem to be still in a developing stage because of the difficulty in treating the nonequilibrium quantum systems. In the previous study, we presented the numerical method, which can treat the non-linear response, making use of a recursive Green-function method based on the Keldysh formalism.[9] Using this method, in the present study, we have performed numerical calculations to investigate the non-linear current-voltage $(I-V)$ characteristics for various sample geometry containing tunnel junction. We have also investigated the effect of the randomness in the insulating layer on the current. We concentrate ourselves on the paramagnetic tunnel junctions for simplicity throughout this work.

2. Model and Method

We consider a metal/insulator/metal trilayer structure, in which the parameter l is introduced as a label of the layer in z-direction. The regions where $l \leq 0$ and $l \geq N+1$ are the semi-infinite metallic leads and the region where $1 \leq l \leq N$ is the insulating layer (central region). The lattice structure of the system is taken to be simple cubic with the lattice constant a and the (001) orientation of the layers is taken as the stacking direction (z-direction). The thickness of the insulating layer is Na and the cross section of the system is $Ma \times Ma$. The periodic boundary conditions are adopted in the $x-$ and $y-$direction. The parameter M is set to be nine in this work. We use a single-orbital tight-binding model with a nearest neighbor hopping term and an on-site delta function-like potential term. The Hamiltonian $\mathcal{H}$ is given as

$$\mathcal{H} = -t \sum_{<(i,l),(i',l')>} (c^\dagger_{i,l} c_{i',l'} + \mathrm{H.c.}) + \sum_{i,l} V_l(\mathbf{r}_i) c^\dagger_{i,l} c_{i,l} + \sum_i \sum_{l=1}^{N} \Phi_l \, c^\dagger_{i,l} c_{i,l} \, , \tag{1}$$

where $\mathbf{r}_i$ and l denote the positional vector in x-y planes and the layer index in z-direction, respectively, and $c^\dagger_{i,l}$ is the creation operator for an electron at the site $(\mathbf{r}_i, l)$. The on-site potential energy $V_l(\mathbf{r}_i)$ depends on atom which occupy the site $(\mathbf{r}_i, l)$. The last term appears when the bias voltage V along the z-direction is applied to the central region (insulating layer), and we assume the electrostatic potential to be $\Phi_l \equiv eV$ in the left lead, and $\Phi_l \equiv 0$ in the right lead. In the central region, for $1 \le l \le N$, it is assumed to be $\Phi_l = eV(N+1-l)/(N+1)$ when the electric field is uniform.

The total current flowing along the z–direction, in which the electric field is applied, can be expressed in terms of the retarded (+) and advanced (-) Green functions[9–11]

$$I_{tot} = \frac{e}{h}\int d\omega\,(f_L - f_R)\,\mathrm{Tr}\,[\boldsymbol{\Gamma}_L\,\boldsymbol{G}^{+}(1,N)\,\boldsymbol{\Gamma}_R\,\boldsymbol{G}^{-}(N,1)]\,, \tag{2}$$

where $f_{L,R} \equiv [e^{(\omega-\mu_{L,R})/k_BT}+1]^{-1}$ with T being temperature μ_L and μ_R being the chemical potentials in the left and right leads with $\mu_L \equiv \mu_R + eV$. k_B is set to be unity. Here Tr denotes the trace for $M^2 \times M^2$ matrices, $\boldsymbol{\Gamma}_L \equiv it^2\left[\boldsymbol{G}_L^{+}(0) - \boldsymbol{G}_L^{-}(0)\right]$, and $\boldsymbol{\Gamma}_R \equiv it^2\left[\boldsymbol{G}_R^{+}(N+1) - \boldsymbol{G}_R^{-}(N+1)\right]$ with $\boldsymbol{G}_L^{\pm}(0)$ and $\boldsymbol{G}_R^{\pm}(N+1)$ being the Green functions for the edge of the unconnected leads on the left and right. $\boldsymbol{G}^{\pm}(l,m)$ is the interlayer Green's function, *i.e.*, an l-m element of the Green's function operator $\mathcal{G} \equiv (\omega \pm i0 - \mathcal{H})^{-1}$. The interlayer Green's functions are calculated numerically by recursive Green's function technique. The detailed description for the calculation of the interlayer Green's function is given in ref 9.

3. Numerical results

Now we discuss the transport phenomena through an insulating layer. In what follows, we take the transfer integral t as a unit of the energy. The origin of μ_R corresponds to $-6t$. For computing the nonequilibrium current, the integral in Eqs. (2) is replaced by the Simpson's sum, and the mesh is taken to be typically $\Delta\omega = 10^{-5}$. We first consider a system including a single impurity inside the insulating layer. The thickness of the insulating layer is set to be $N = 3$ in this single impurity case. We take the on-site potential energy $V_l(\mathbf{r}_i) = 0$ for $l \le 0, l \ge 4$. Inside the insulating barrier $(1 \le l \le 3)$, $V_l(\mathbf{r}_i)$ is chosen to the barrier height $7t$, except the impurity site. At the impurity site, $V_l(\mathbf{r}_i)$ is taken to be zero. The position of the impurity in z direction is the center of the insulating layer, *i.e.*, $l = 2$. We have calculated the total current as a function of μ_R for various temperatures as shown in Figs. 1 (a) and (b). As can be seen from Fig. 1 (a) a sharp peak appears at $\mu_R = 5.1$ and $T = 0$ for the linear response case at $eV = 0.001$. This is due to the resonant tunneling occurring through a local energy level constructed by the single impurity, which becomes broader as the temperature increases. In the non-linear response case (at $eV = 0.5$), where $I - V$ characteristic is non-linear, the structure of the peak changes considerably, as shown in Fig. 1 (b) at $T = 0$. In this single impurity system, the most current flows through the local impurity, and hence, the total current remains unchanged during the local impurity level lies between μ_R and μ_L. In other word, the value of the trace in eq. 2 is almost constant in this case. In this $T = 0$ case, the current becomes approximately

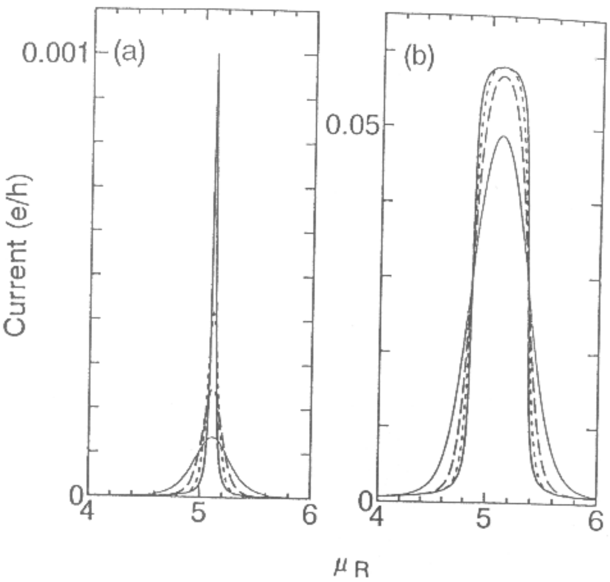

Fig.1 μ_R dependence of the current for the single impurity case. The bias voltage eV applied is (a) 0.001 and (b) 0.5. The thick solid, dotted, dashed, and thin solid curve represent the calculated current at $T = 0, 0.025, 0.05$ and 0.1, respectively.

$$\begin{aligned} I_{tot} &\approx \frac{e(\mu_L-\mu_R)}{h}\,\mathrm{Tr}\,[\boldsymbol{\Gamma}_L\,\boldsymbol{G}^{+}(1,N)\,\boldsymbol{\Gamma}_R\,\boldsymbol{G}^{-}(N,1)] \\ &= \frac{e(\mu_L-\mu_R)}{h}\,\mathrm{Tr}\,(\,\boldsymbol{t}\,\boldsymbol{t}^{\dagger}\,)\ , \end{aligned} \tag{3}$$

where $\boldsymbol{t}$ is the transmission matrix through the insulating layer. Since $\mathrm{Tr}\,(\,\boldsymbol{t}\,\boldsymbol{t}^{\dagger}\,)$ is approximately constant due to the single resonance, $I_{tot} \sim e(\mu_L - \mu_R)/h \times$ const., if the impurity level exist between μ_R and μ_L, otherwise $I_{tot} \sim 0$. Therefore, we can see the nearly rectangle shape in the current curve at $T = 0$ [see Fig. 1 (b)]. As the temperature increases, the shape of the current curve gradually approaches that seen in Fig. 1 (a) at $T = 0.1$ [see Fig. 1 (b)], although the peak values of the current differ greatly. We also shows the μ_R dependence of the current at $T = 0$ for various bias voltages in Fig. 2. As the bias voltage increases, the peak becomes broader, and finally the rectangle shape can be seen.

Next, we discuss the tunnel conduction through an insulating layer containing random impurities. We use the simple model for considering the randomness which can be seen in the experiment. In the present case, the location of the impurities in the insulating layer are determined by the uniform random numbers. The thickness of the insulating layer is taken to be N=5 in the following calculations. We take the on-site potential energy

$V_l(\mathbf{r}_i) = 0$ for the impurity again and the impurity concentration is $c = 0.1$.

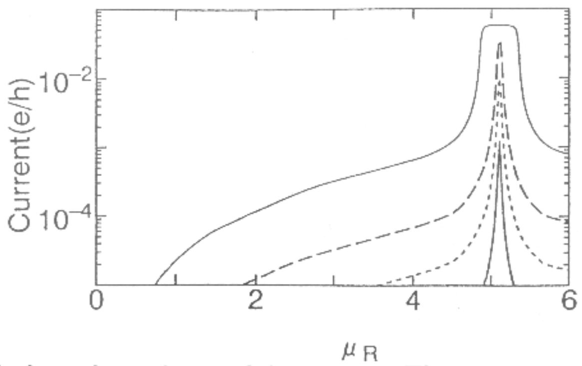

Fig.2 μ_R dependence of the current. The current scale in the vertical axis is made logarithmic. The applied bias voltage eV is (a) 0.001 and (b) 0.5. The thick solid, dotted, dashed, and thin solid curves show the calculated currents at $eV = 0.001, 0.01, 0.05$ and 0.5, respectively.

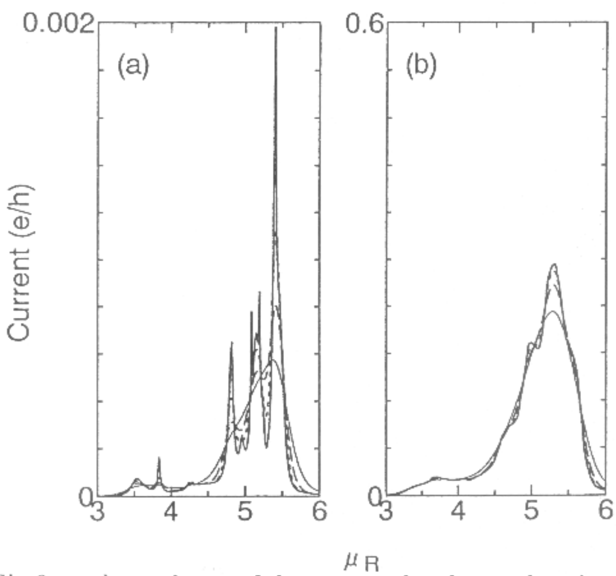

Fig.3 μ_R dependence of the current for the random impurity case. The bias voltage eV applied is (a) 0.001 and (b) 0.5. The thick solid, dotted, dashed, and thin solid curves represent the calculated currents at $T = 0, 0.025, 0.05$ and 0.1, respectively.

Figures 3 (a) and (b) give the typical examples of the μ_R dependence of the current for (a) $eV = 0.001$ and (b) $eV = 0.5$ at $T = 0, 0.025, 0.05, 0.1$ in the random impurity cases. The position of the impurity sites are same in both cases. In the linear response case at $eV = 0.001$ [see Fig. 3 (a)], sharp current peaks can be seen, which is due to the resonant tunneling by the impurity levels. This sharpness of the peak structure of the current curve disappears rapidly with increasing temperatures [see Fig. 3 (a)]. The peak positions can be determined by the relative location of the impurities. In the non-linear response case at $eV = 0.5$, the shape of the curve structure of the current even at $T = 0$ resembles that seen in Fig. 3 (a) at $T = 0.1$. This feature is much different from that in the single impurity case. The curve structure at $T = 0$ in $eV = 0.5$ is almost kept at $T = 0.1$. At $T = 0$ in the non-linear case at $eV = 0.5$, many impurity levels are present between μ_L and μ_R so that the averaging takes place by the summation of the currents contributed from many impurity levels. Hence in this case of random multi-impurity levels the effect of the increase of the bias voltage on the curve structure resembles that of the temperatures.

4. Summary

In summary, we have investigated the transport phenomena through a tunnel junction containing impurity atoms. We have investigated the bias voltage and temperature dependence of the non-linear $I-V$ characteristics by using the recursive Green function method. We have found that the effect of the temperature on the tunnel current in the non-linear $I-V$ characteristics is smaller than that in the linear-response case. We also found that the peak shape of the current at $T = 0$ and $eV = 0.5$ for the single impurity case is much different from that for the random impurity case.

This method can be extended for investigating TMR and the result of the study on the effect of the bias voltage and temperature on TMR will be presented elsewhere.

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