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Kondo effect for electron transport through an artificial quantum dot*

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We have calculated the transport properties of electron through an artificial quantum dot by using the numerical renormalization group technique in this paper. We obtain the conductance for the system of a quantum dot which is embedded in a one-dimensional chain in zero and finite temperature cases. The external magnetic field gives rise to a negative magnetoconductance in the zero temperature case. It increases as the external magnetic field increases. We obtain the relation between the coupling coefficient and conductance. If the interaction is big enough to prevent conduction electrons from tunnelling through the dot, the dispersion effect is dominant in this case. In the Kondo temperature regime, we obtain the conductivity of a quantum dot system with Kondo correlation.

Keywords: Kondo effect, quantum dot, numerical renormalization group
PACC: 7320D, 7340G, 7340C, 7170G

1. Introduction

Recently in calculating the transport problems of the quantum dot system, the numerical renormalization group(NRG) method[1] has been employed. Hofstetter[2] developed the NRG method to the reduced density matrix-NRG method. It has been used in the Anderson impurity model in an external magnetic field, which is interesting to us in view of recent transport properties measurements of quantum dot(QD) system.[3] The QD acts as a magnetic impurity. So it builds up correlated Kondo-like states[4−7] and causes conductance fluctuation. All electrons are tight-bound in the semiconductor quantum dot system except a small number of free electrons which can range from zero to several thousands.[8] In this paper, we employ the s-d exchange model to obtain Kondo Hamiltonian. The simplest physical model is a one-dimensional lead which is embedded in a QD with a single electron at the lowest level. A single electron transports through the QD (ie. we restrict the subspace $\vec{S} = 1/2$) and the low-energy behaviours of transport can be obtained by using the Fermi liquid theory. We only consider one electron on the dot in order to simplify the model. In the previous works, the focus of research is Kondo correlations and Coulomb blockade phenomena. The NRG calculation[9] was applied in Anderson impurity model[10] and Aharonov–Bohm (AB) interferometer. The result of a plateau of ϕ in the Kondo valley was given in Ref.[11]. Our work has been concentrated on the Kondo effect and transport behaviours of a quantum dot system.

In this paper, we use the Kondo model to investigate the transport behaviours of a quantum dot system in zero and finite temperature cases by using the Green function (GF) method. Here, we define a GF of the charge part by imitating the GF of the spin lattice of a ferromagnet. It is convenient to obtain some transport characters of mesoscopic circuits. We observe the negative magnetoconductance at zero temperature. In the finite temperature case, as the external magnetic field increases, the maximum of conductance seems to occur at an approximately fixed temperature. It is the Kondo temperature ($T_{\rm K}$) that is determined by the coupling coefficients. In this region, the Kondo peak appears noticeably. In Fermi liquid

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theory, spin and charge are entangled, and we consider that they are two channels. The spin part represents impurity spin (namely the impurity electron number of occupation on dot), and the charge part (namely orbital pseudospin) the electron number of the lead part.[3] But only the charge part contributes to the tunnelling conductance. We also calculate for the cases of different couplings which affect the results of tunnelling conductance in zero-temperature regime. When the coupling is strong enough, the transport conductance tends to zero. In this case, the dispersion process is dominant.

2. The model and basic formulae

We consider a one-dimensional chain in which a quantum dot is embedded.[13] We suppose the QD has a spin impurity coupling with the electrons of leads. Here we study the case that there is only one electron on the QD (namely the spin 1/2 Kondo model). The simple model is convenient for understanding some transport behaviours. The Hamiltonian can be written as:

$$H_{\rm dot} = -BS_Z\left(\frac{1-T_Z}{2}\right) + \frac{U}{2}(T_Z+1)\left(\frac{\sigma_Z+1}{2}\right) + eV_{\rm g}\left(\frac{1-T_Z}{2}\right) + 2eV_{\rm g}\left(\frac{T_Z+1}{2}\right)\left(\frac{\sigma_Z+1}{2}\right). \quad (1)$$

In the dot, we only consider the Zeeman splitting due to an applied local magnetic field B in the Z direction. We tune the gate voltage $V_{\rm g}$ in order to keep the zero potential energy of the dot. S_Z represents the Z direction spin. U is the Coulomb energy. The operation $T_Z = -1$ represents odd occupation case on the dot, and $T_Z = 1$ the even occupation or empty occupation. So only one operation T_Z cannot distinguish the even from the empty case. We must give a new operation σ_Z to discriminate the two phases. When $\sigma_Z = -1$, it represents the empty case, and $\sigma_Z = 1$ the even occupation, where the lead term is expressed by the Hamiltonian

$$H_{\rm leads} = \sum_{k\sigma r} \epsilon_{k\sigma r} a^+_{k\sigma r} a_{k\sigma r}, \quad (2)$$

where $a^+_{\epsilon\sigma}(a_{\epsilon\sigma})$ creates an electron in the right (left) lead with energy ϵ and spin σ, D is the half bandwidth (here we set D=1), and there is an anticommunication relation between them. Then the coupling terms are described by s-d exchange interaction, assisting the tunnelling and orbital pseudospin interaction.[3] They are written in the following effective Hamiltonians:

$$H_{\rm Kondo} = J\left(\frac{1-T_Z}{2}\right)\boldsymbol{S}(\psi^+\boldsymbol{\sigma}\psi), \quad (3)$$

$$H_{\rm assist} = Q_\perp\left(\frac{1-T_Z}{2}\right)[\boldsymbol{S}(\psi^+\boldsymbol{\sigma}\tau^-\psi) + {\rm h.c.}], \quad (4)$$

$$H_{\rm orb} = \frac{1}{2}V_\perp[\psi^+\tau^-\psi + {\rm h.c.}], \quad (5)$$

where $\psi \Longrightarrow$

$$\psi_{\sigma\tau} = \int a_{\varepsilon\sigma\tau}\,{\rm d}\varepsilon,$$

$\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ represent the spin and the orbital pseudospin of the electrons on the lead, and $\boldsymbol{S}$ is the spin of the electrons of the dot. $\tau = 1(-1)$ denotes the electrons in the right (left) lead. Here, we consider it as the orbital pseudospin Pauli matrix. These effective Hamiltonians are perturbation terms in the lead-dot tunnelling process.[1] J is the coupling of impurity and conductive electrons, and $J \sim \Gamma$, Γ being the tunnelling rate to the lead. In the assistance term, T^+ is the generation operation of the orbital pseudospin of the impurity electron. Here, τ^- annihilates the lead electrons. So this term represents the tunnelling process. $Q_\perp \sim \Gamma$(assuming the action symmetry, Γ_+ is equal to Γ_-). The last term is the orbital Kondo part, and $V_\perp \sim Q_\perp$. The total Hamiltonian of the system is written as: $H_{\rm int} = H_{\rm dot} + H_{\rm Kondo} + H_{\rm assist} + H_{\rm orb}$.

3. Numerical renormalization group

Wilson's NRG method is convenient for studying Kondo problem. Using the approach, we can access to the transport behaviours of the one-dimensional chain under the low temperature condition. We calculate the Hamiltonian by the level calculation procedure. First, we define a series of rescaled Hamiltonians H_N. They are written as[1]

$$H_{N+1} = \Lambda^{1/2}H_N + \sum_{\sigma\tau}\xi_N(f^+_{N+1\sigma}f_{N\sigma} + f^+_{N\sigma}f_{N+1\sigma}), \quad (6)$$

where $f_{0\sigma\tau} = \psi_{\sigma\tau}/\sqrt{2}$ and $H_0 = 2\lambda^{1/2}/(1+\lambda)H_{int}$. Here we let $\lambda \sim$3. The successive conduction band [–1, 1] is now discretized. Λ is a discretion parameter with a real space scale. In momentum space, the wave vector k is discretized by $\frac{1}{\Lambda^N}$, and N is the iteration step. Then the relation between the original Hamiltonian H and the defined rescaled Hamiltonian is $H = \lim_{N\to\infty}\omega_N H_N$, and $\omega_N = \Lambda^{-(N+1)/2}(1+\Lambda)/2$. We iteratively diagonalize Eq.(6), then the level spectrum can be obtained in the low temperature case.

In order to obtain matrix elements of H_0, we need to define a tentative wave function. It reads:

$$\Phi_0 = \sum_{\sigma\tau}(f^+_{0\sigma\tau}|vac\rangle|\uparrow\rangle + f^+_{0\sigma\tau}|vac\rangle|\downarrow\rangle). \quad (7)$$

The basis used for H_{N+1} is the product basis of eigenstates $|p,i,\tau\rangle$. $|i,\tau\rangle$ is the state of site $N+1$ (i.e. $|i,\tau\rangle = |0,\tau\rangle, |\uparrow,\tau\rangle, |\downarrow,\tau\rangle$ and $|\uparrow,\downarrow\tau\rangle$, $\tau = \pm 1$, total 8 states) and $|p\rangle$ is the eigenstate of H_N. It is written as $|p\rangle = \sum_{r,i,\tau} U_N(p, ri\tau)|r\rangle_{N-1}\ |i,\tau\rangle$, where $|r\rangle$ denotes an eigenvector of the foregoing cluster $(N-1)$, but here $|i,\tau\rangle$ is the state of site N. $U_N(p,ri\tau)$ is the matrix of eigenvectors of H_N. Under these conditions, we obtain the matrix elements of H_{N+1} in this assuming basis. They are written as

$$\begin{aligned}&\langle p, i\tau|H_{N+1}|q, j\tau'\rangle\\ =&\Lambda^{1/2}\delta_{p,q}\delta_{i,j}\delta_{\tau,\tau'}E^N_p\\ &+\sum_{\sigma\tau\tau'}\xi_N(-1)^N(\langle i\tau|f^+_{N+1\sigma\tau}|j\tau'\rangle\langle p|f_{N\sigma\tau}|q\rangle\\ &+\langle i\tau|f_{N+1\sigma\tau}|j\tau'\rangle\langle p|f^+_{N\sigma\tau}|q\rangle), \quad (8)\end{aligned}$$

$$\begin{aligned}\langle p|f_{N\sigma\tau}|q\rangle_N =&\sum_{r,i\tau}\sum_{r',j\tau'}U^*_N(p,ri\tau)U_N(q,r'i'\tau')\\ &\times\delta_{r,r'}(-1)^{N-1}\langle i\tau|f_{N\sigma\tau}|j\tau'\rangle. \quad (9)\end{aligned}$$

Using the iterative diagonalization result, we can obtain the low energy eigenvalues and eigenstates of this system. The transport characters can be calculated at a scale $T_{\rm K}$, $\omega \sim \omega_N$. Now we define a Green function about orbital pseudospin. It reads:

$$\begin{aligned}G_\tau =&\sum_{\sigma\sigma'}\langle\langle\tau^-;\tau^+\rangle\rangle_{\omega+i\eta}\\ =&\sum_{\sigma\sigma'}\langle\langle f^+_{0\sigma(-1)}f_{0\sigma(+1)};f^+_{0\sigma'(+1)}f_{0\sigma'(-1)}\rangle\rangle_{\omega+i\eta}.\end{aligned} \quad (10)$$

The Kubo expression for the conductance is

$$G = \frac{2e^2}{h}\lim_{\omega\to 0}\frac{\rho^y_\tau(\omega)}{\omega}, \quad (11)$$

where $\tau = \pm 1$ represents the orbital pseudospin of the right (left) lead, and $\rho^y_\tau(\omega)$ is the pseudospin spectral function which is derived from the defined Green function.

$$\rho^y_\tau(\omega) = -\frac{1}{\pi}{\rm Im}G_{\sigma\sigma'}(\omega). \quad (12)$$

This conductance formula can be used in both zero and finite temperature cases.[3]

4. Numerical results

First we calculate for the zero temperature case. The Green function at zero temperature can be written as

$$G_\tau(\omega) = \sum_{\sigma\sigma' n}\frac{\langle 0|f^+_{0\sigma(-1)}f_{0\sigma(+1)}|n\rangle\langle n|f^+_{0\sigma'(+1)}f_{0\sigma'(-1)}|0\rangle}{\omega-\omega_{n0}+i\eta}, \quad (13)$$

where $\omega_{n0} = \frac{1}{\hbar}(\varepsilon_n - \varepsilon_0)$. It represents transition between energy levels. Here, we only use the part of $\omega > 0$. Using Eq.(13), we calculate the conductance at T=0K. Thus we obtain Fig.1, which shows the relation between conductance and external magnetic field (i.e. the G–B curve). We observe the expected large negative magnetoconductance which increases with increasing magnetic field. This can be clearly seen from Fig.1. We can employ the Nth shell to calculate the conductance. The character of the G–B curve is similar to the result of László *et al.*[3] We must stress that the magnetoconductance quickly reaches a saturated value in the small Zeeman splitting case, as can be seen from Fig.1. The electron of the impurity has two spin directions(we consider that they are two channels). In no external magnetic field case, the level is degenerative. As B increases, the degeneracy disappears and the level gap increases. In the Nth shell, the reliable range of the energy is $\omega_N \le \omega \le 10\omega_N$.[2] Here, we use the $\omega \sim 2\omega_N$. This is a simple conductance calculation method, and the Kubo expression is adapted in the zero and the infinite temperature cases. At zero temperature, another relation we obtain is the change of the conductance as the coupling coefficient increases. In Fig.2, it can be seen that the conductance quickly decreases to zero as the coupling increases. It is caused by the electron coherent phase. When the coupling coefficient is strong enough, the dispersion is dominant, and the conductance is approximately equal to zero. As J increases, the conduction electron is scattered by the electron of the impurity more intensively. The conduction process is prevented by the scattering process. We find that the conductance is not a consecutive drop as the Kondo coupling coefficient increases. In the system,

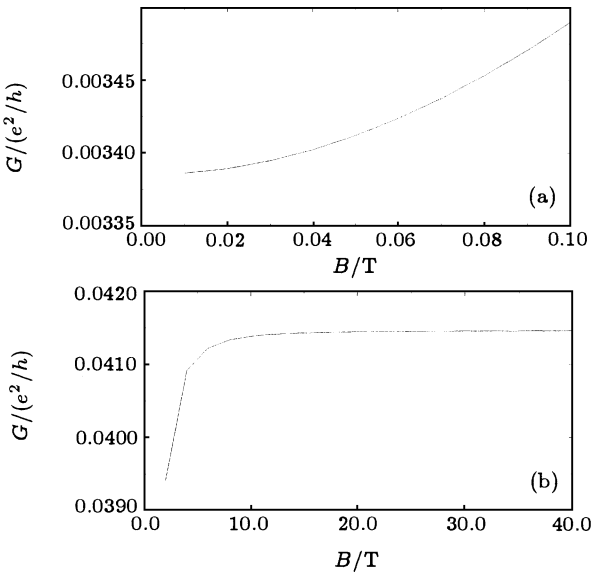


Fig.1. The T=0K conductance of the quantum dot system at $\omega \sim \omega_N$ for $J = 0.14, Q_\perp = V_\perp = 0.13, \epsilon = -0.1$. (a) $B = 0.01-0.1$T for small magnetic field case. (b) $B = 2-40$T for big magnetic field case. The curve represents the variation of negative magnetoresistance with increasing magnetic field. In our calculation, the conductance of the system changes very quickly below 5.0T. Beyond 5.0T, the conductance quickly reaches a saturated value.

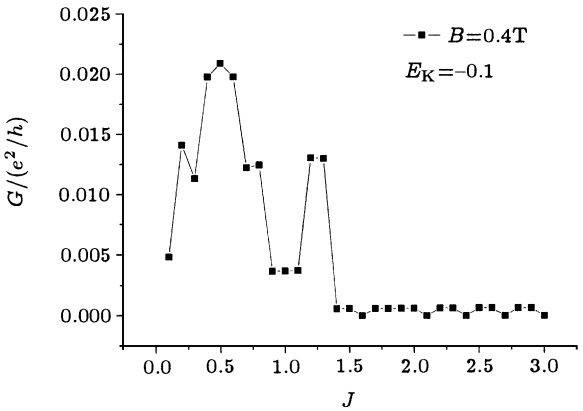


Fig.2. The relation between the pseudospin coupling and the conductance. In this case, $B = 0.4, V_\perp = Q_\perp \simeq J \sim 0$ to 3.0, and $\epsilon = -0.1$. It can be seen that the conductance of the system is oscillating when J is below 1.4.

the phase changes as the Kondo coupling varies. It brings up the coherent condition. So the result in Fig.2 represents a competition process of the strong dispersion and the coherent condition. Some physical properties can be derived from the finite temperature Green function. Here, we give the finite temperature conductance formula: $G(T) \sim \lim_{N\to\infty} \frac{\rho_\tau^N(\omega,T)}{\omega}$, where the finite temperature spectral density is written as:

$$\rho_\tau^N(\omega,T) = \frac{1}{Z_N(T)} \sum_{\sigma\sigma'} \sum_{\mu} \exp(-E_\mu/T)\delta(\omega - E_\mu + E_v)\langle\mu| f^+_{0\sigma'(+1)} f_{0\sigma'(-1)} |v\rangle\langle v| f^+_{0\sigma(-1)} f_{0\sigma(+1)} |\mu\rangle. \quad (14)$$

Here, $Z_N(T)$ is the partition function, and $|\mu\rangle$ are the many-particle eigenstates of H. We have adopted units as $\hbar = k_b = g = \mu_B = 1$. We know that the number of iterations corresponds to the temperature in NRG, and it is given by $T_N = c\Lambda^{-(N+1)/2} \sim \omega_N$. Here c is a constant that can be tuned. In the Kondo temperature region, the spectral density at a certain temperature can be calculated by using the shell spectrum densities $\rho_\tau^N(\omega,T)$ at the frequencies $\omega_N \le \omega \le 10\omega_N$ when $\Lambda = 3$.[2] It restricts the reliable range of excitations ω because of the truncation of the spectrum in H_N. We use the Nth shell in which $T_N \sim T_K$, and c can change approximately from 10 to 100 in this energy shell (we assume that the temperature range is $10\omega_N - 100\omega_N$, which is adapted to the requirement of $T_K \le T \le 10T_K$,[12] and ω_N is the lowest scale of H_N). We obtain the finite temperature conductance for the case of different magnetic fields in Fig.3. In these conductance figures, it can be found that T_K (Kondo temperature) changes inconspicuously as the magnetic field alters. This result is in accordance with $T_K = D|2J\rho|^{1/2}exp(-1/|2J\rho|)$($\rho$ represents the density of states at the Fermi surface).[1] In Fig.3, $T_K \sim 30\omega_N$ is the temperature of the Kondo peak.

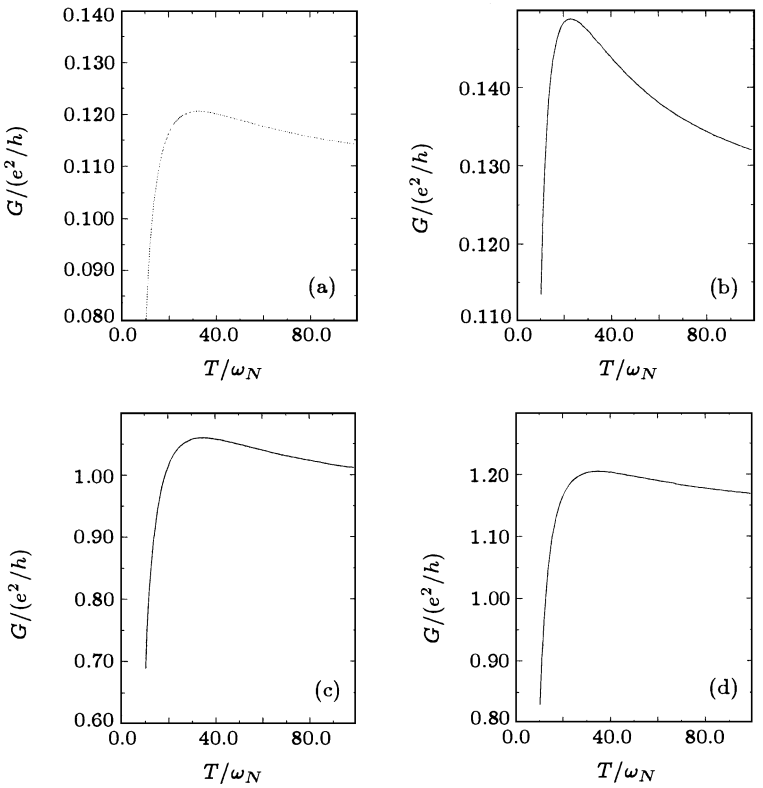


Fig.3. Here, $T_{\rm K} \sim 30\omega_N$. (a) Conductance for $J = 0.14, Q_\perp = V_\perp = 0.13, B = 0.4$, and $T = 10\omega_N - 100\omega_N$. Here, we obtain the known Kondo peak. (b) The difference is $B = 0.8$. The Kondo peak is more obvious. (c) $B = 1.6$. (d) $B = 3.2$. The conductance reaches the maximum at $T \sim 30\omega_N$, and we consider it as the Kondo temperature.

5. Conclusion

In this paper, we have studied the transport behaviours of the Kondo impurity system by using the NRG method. We define the zero temperature and the finite temperature using Green function in order to calculate the conductance by using the Kubo expression for the conductivity. In the zero temperature case, we observe the negative magnetoresistance by calculating for conductance at a scale ω_N(ie. the Nth shell). And the influence of the coupling on conductance is also studied at zero temperature. In the system, we observe that there are two effects: One is the dispersion effect which suppresses the electron tunnelling at strong coupling, the other is the coherent effect which generates the resonance of the tunnelling conductance. Finally, we calculate the finite temperature conductance, and obtain the Kondo effect in the Kondo temperature regime.

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