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Numerical study of the electrical conductivity of a low-dimensional Kondo lattice model

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Abstract

We investigated electron transport in ladder-structured Kondo lattice models with antiferromagnetic coupling between localized $S = 1/2$ spins. In a system where two spins on the ladder rung dimerize, conductivity shows an anomalous non-monotonic field dependence in contrast with ordinary magnetoresistance. This is attributed to a spin configuration that is represented by a product of singlets and triplets on the ladder rungs. However, when the spin exchange interactions of the Heisenberg-type are considered between two spins on diagonals in the ladder, such a spin configuration is destroyed and the non-monotonic field dependence is dissolved.

1. Introduction

In conventional electronics, many devices are controlled by an electron charge. Recently, extensive investigations have been carried out in order to utilize another property of electrons, namely spin. If the lead of a device is made of some magnetic material it is plausible that the electrical resistivity of the lead is determined by an interaction between spins of conduction electrons and localized spin in the lead. The localized spins connected by magnetic interactions show various magnetic orderings depending on the geometrical structure of the spin network. In theoretical investigations, the Kondo lattice model is often used to study the effect of electron scattering by magnetic impurities. We have investigated the effects of magnetic ordering on electron transport as revealed by the model with antiferromagnetic spin couplings [1]. We use linear response theory and evaluate static conductivity with the Kubo formula [2, 3], which is obtained as [4, 5]

$$\sigma_{\mu\mu} = \langle K_\mu \rangle + \frac{\beta}{Z} \sum_{m,n} \mathrm{e}^{-\beta E_m} \, |\langle m| \, J_\mu \, |n\rangle|^2 \, \delta \left(E_n - E_m \right) . \tag{1}$$

Here, K_μ and J_μ are, respectively, the kinetic-energy and current operators in direction μ. β is the inverse temperature, $1/T$, and $Z = \sum_m e^{-\beta E_m}$. In a system where the localized $S = 1/2$ spins form an antiferromagnetically coupled two-leg ladder, whose Hamiltonian is given by equations (2) and (3) with $J_{\rm diag} = 0$, we observed an anomalous behaviour of conductivity [1]. When the ladder-rung interaction is sufficiently strong compared to the ladder-leg one, it shows non-monotonic field dependence in contrast with an ordinary magnetoresistance where conductivity shows a monotonic increase with magnetic field, which is shown by *solid* curves in figures 2(a) and (b). Here, in the first term on the right-hand side of equation (3), we set the exchange interactions on the ladder legs as the Ising-type. However, even if they are the Heisenberg-type, non-monotonic behaviour is clearly observed, although it is less remarkable. It is considered that this anomalous behaviour is attributed to a spin configuration of localized spins that is represented by a product of spin singlets and triplets on the ladder rungs, as shown in figure 1. In the system, as the ladder-rung interaction is strong, a spin singlet pair is formed on each ladder rung at zero field. Then, an antiferromagnetic ordering along the ladder leg is destroyed, which results in high zero-field conductivity since hopping of conduction electrons causes almost no energy loss in spite of spin-electron interaction, $J_{\rm H}$. However, as the magnetic field increases, some of the singlets turn into triplets. A spin in a triplet has a different polarization from that in a singlet. Then, conduction electrons with a spin parallel to a triplet can hop less freely from the triplet- to the singlet-rungs. Of course, ferromagnetic ordering yields high conductivity. As a result, the spin configuration at each field leads to a dip in conductivity. In this manner, quantum property in the localized spin system causes interesting behaviour of conductivity, and it is expected that such a behaviour changes sensitively depending on the magnetic structure of the system. In this paper we report the effects of additional terms that play an important role in determining the magnetic structure. We consider diagonal paths on the ladder: exchange interaction between two localized spins on a diagonal in the ladder and electron transfer between two diagonal sites.

2. Results

Now, we consider a system in which the localized spins couple antiferromagnetically on the ladder with diagonal paths and an external magnetic field is applied on the system, whose Hamiltonian is given by

$$\mathcal{H} = \mathcal{H}_{\rm ex} - 2J_{\rm H}\sum_k\sum_\sigma S_k^z\sigma c_{k,\sigma}^\dagger c_{k,\sigma} - t\sum_{\langle k,l\rangle}\sum_\sigma\left(c_{k,\sigma}^\dagger c_{l,\sigma} + c_{l,\sigma}^\dagger c_{k,\sigma}\right) - H\left(\sum_k S_k^z + s^z\right) \tag{2}$$

where

$$\begin{aligned}\mathcal{H}_{\rm ex} = & -2J_{\rm leg}\sum_{i=1}^{4}\sum_{j=1}^{2} S_{i,j}^z S_{i+1,j}^z - 2J_{\rm rung}\sum_{i=1}^{4}\boldsymbol{S}_{i,1}\cdot\boldsymbol{S}_{i,2} \\ & -2J_{\rm diag}\sum_{i=1}^{4}\left(S_{i+1,1}^x S_{i,2}^x + S_{i+1,1}^y S_{i,2}^y + A_{\rm diag}S_{i+1,1}^z S_{i,2}^z\right).\end{aligned} \tag{3}$$

The relationship between spins and bonds is shown in figure 1. Here S_k^x, S_k^y and S_k^z are the x-, y- and z-components, respectively, of the total spin operator of the localized $S = 1/2$ spin at site k, $\boldsymbol{S}_k$. Here, k or l in equation (2) represent a combination of rung index i and leg index j in $\boldsymbol{S}_{i,j}$ which are used in equation (3) and figure 1. s^z is the z-component of the

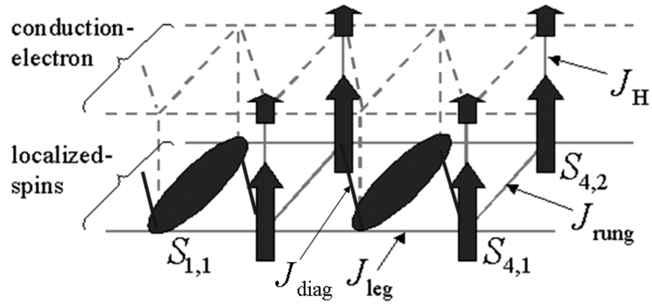

Figure 1. Schematic structure of the spin configuration and electron distribution in the ladder-structured Kondo lattice model with $J_{\mathrm{diag}} = 0$. Upper and lower ladders correspond to the area of conduction electron and localized spins, respectively. The shaded ellipsoid and long arrow represent a singlet of two spins and a localized spin, respectively. The shaded short arrow represents a spin of electron whose on-site probability is $1/4$ due to its distribution.

electron spin, and $c^{\dagger}_{k,\sigma}$ and $c_{k,\sigma}$, respectively, create and annihilate the conduction electron with magnetization σ $(= \pm 1/2)$ at k. In this work, we adopt a system in which the two-leg ladder consists of 4 rungs, namely 8 sites, and use a periodic boundary condition. We consider a low electron-density limit of single-electron conduction. We set J_{H} as ferromagnetic. Localized spins interact with each other via three types of antiferromagnetic bond, namely ladder-rung, ladder-leg and diagonal bonds. For simplicity, we set the transfer integrals to have the same values for the ladder rung, the ladder leg and the diagonal as shown in the third term on the right-hand side of equation (2), where $\langle k, l \rangle$ counts for all bonds on which the exchange interaction is considered. Here, we set the current direction parallel to the ladder leg. We adopt the parameters, except for on-diagonal exchange and transfer integrals, that are the same as those used in the previous work on a pure ladder system. In figure 2, we show the field dependences of conductivity at sufficiently low temperature. Figure 2(a) corresponds to the case where the on-diagonal exchange integral is the Ising-type, namely $A_{\mathrm{diag}} = \infty$, and (b) the Heisenberg-type, $A_{\mathrm{diag}} = 1$. In each figure, we change the amplitude of the on-diagonal exchange integral from 0 to -20 K. Although the diagonal bond causes a frustration in the ladder, since the bond is sufficiently weak compared to the rung bond, we do not have to consider the effect. However, an anisotropy of the diagonal bond plays an important role. In figure 2(a) for $A_{\mathrm{diag}} = \infty$, the dip in the middle range of the magnetic field remains. The Ising exchange integral connects spins classically and then, except for the effect of the frustration, the structure given by a product of on-rung singlets and triplets is preserved and each rung still independently turns from singlet to triplet. Then, the dip structure remains following the picture explained in the previous section. On the other hand, in figure 2(b) for $A_{\mathrm{diag}} = 1$, the dip is going to disappear as the diagonal bond is strengthened. In contrast with the classical case, the localized spins are connected by the rung- and the diagonal-bonds into a one-dimensional zigzag structure and the spin chain shows a quantum fluctuation. Then, the independence of the rung is lost and the singlet–triplet structure is destroyed. In the result, the dip structure is dissolved. This change suggests that, for example, when a system shows a pressure-induced distortion and there occur additional exchange paths, the behaviour of conductivity may qualitatively change. In addition, from these results on two types of the diagonal bond, we can see that the behaviour of conductivity is very sensitive to a spatial anisotropy of the system. It is expected that, in systems with a specific spatial anisotropy, we can observe such an anomalous non-monotonic field dependence of conductivity.

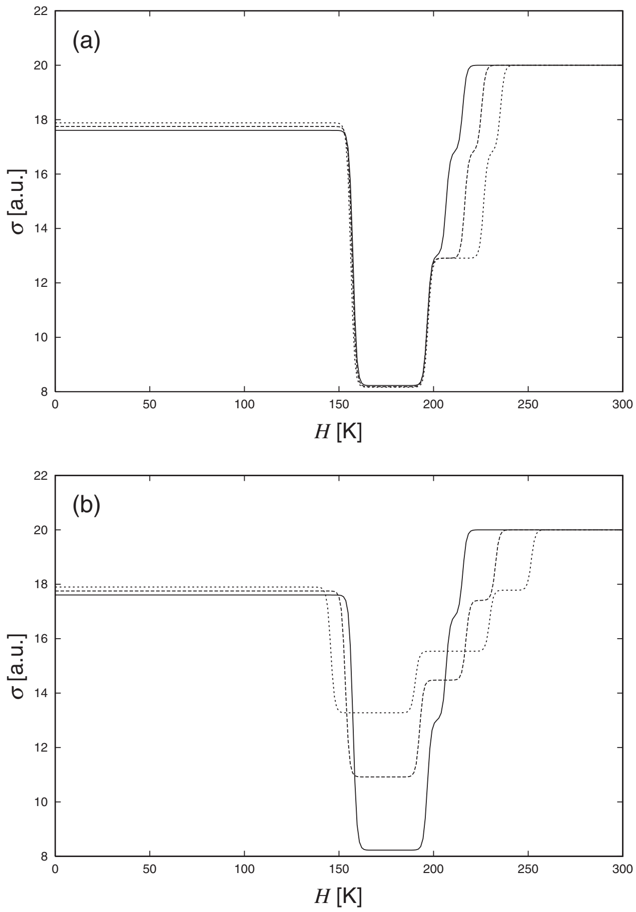

Figure 2. Field dependences of conductivity of the ladder system with various on-diagonal exchange integrals at $T = 1$ K. We set $J_{\rm H} = 200$ K, $t = 10$ K, $J_{\rm leg} = -10$ K, $J_{\rm rung} = -100$ K. In each figure, solid, dashed and dotted curves correspond to $J_{\rm diag} \cdot A_{\rm diag} = 0, -10$ K and -20 K, respectively. (a) $A_{\rm diag} = \infty$ and (b) $A_{\rm diag} = 1$.

3. Summary

We studied the static electrical conductivity of the ladder-structured Kondo lattice model with antiferromagnetic spin couplings. In order to study the dependence of conductivity on the magnetic structure of the localized spin system and the effect of spatial anisotropy, we studied conductivity of the ladder systems with diagonal bonds of the Ising- and the Heisenberg-types. We observed a clear difference between the two cases and obtained proper results which are consistent with the picture for the non-monotonic field dependence. The observed non-monotonic field dependence of conductivity is explained by the formation of singlets and triplets on the ladder rungs. We believe that this type of anomaly is observed in systems with strong spatial anisotropy. We surmise that interchain or interplane quantum properties produce rich and varied characteristics such as high electrical conductivity at zero field, even in antiferromagnets.

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