Magnetoresistance in the s-d Model with Arbitrary Impurity Spin

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Abstract

The magnetoresistance, the number of the localized electrons, and the s-wave scattering phase shift at the Fermi level for the s-d model with arbitrary impurity spin are obtained in the ground state. To obtain above results some known exact results of the Bethe ansatz method are used. As the impurity spin \( S = 1/2 \), our results coincide with those obtained by Ishii et al. The comparison between the theoretical and experimental magnetoresistance for impurity \( S = 1/2 \) is re-examined.

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1. Introduction

The magnetoresistance for the impurity spin \( S = 1/2 \) at temperature \( T = 0 \) was obtained in the s-d model by many authors [1]-[4]. For arbitrary impurity spin \( j \) at \( T = 0 \) the magnetoresistance was obtained in the Coqblin-Schrieffer model [5] (for reviews see [6] and [7]). The purpose of this paper is to study the magnetoresistance for higher impurity spin in the s-d model in the ground state. The electric resistivity obtained by us are given below in (11)-(12). For impurity spin \( S = 1/2 \), (12) coincides with the known result [1]-[4]. We also make a comparison of the electric resistivity for \( S = 1/2 \) with experimental data obtained by Felsh et al. [8]. The same comparison was also done by [5]. Our result is different from that of [5] as shown below in Fig. 1.

2. Numbers of localized electrons, scattering phase shifts and magnetoresistance

The s-d exchange Hamiltonian for an impurity spin \( S \) localized at the origin is

\[
\hat{H} = \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{J}{2} \sum_{k,k',\sigma,\sigma'} c_{k\sigma}^\dagger \sigma \sigma' c_{k'\sigma'} \cdot \mathbf{S},
\]

where \( c_{k\sigma} (c_{k\sigma}^\dagger) \) is the annihilation (creation) operator for an electron with wave vector \( k \) and spin \( \sigma \), \( \varepsilon_k \) is the kinetic energy of the electron with wave vector \( k \),
$S$ is the impurity spin, $\sigma$ is the Pauli matrix, and $J$ is the coupling constant. We will only consider the case of antiferromagnetic coupling ($J > 0$). We can also introduce a magnetic field $H$, then a Zeeman term should be added to the right hand side of (1).

In the ground state, as the impurity spin $S = 1/2$, Yosida and Yoshimori calculated the numbers of the localized electrons around the impurity. Through the Friedel sum rule they obtained the scattering phase shift at the Fermi level and then the magnetoresistance [3] (see also a more succinct presentation [9]). In this work we will generalize the study of Yosida and Yoshimori to the case of arbitrary impurity spin. We assume that certain results of the Bethe ansatz method in one dimensional space [10] can be applied to the s-wave electrons with the above Hamiltonian (1). Under this assumption, the deduction is dramatically simplified.

If the magnetic field $H = 0$, Mattis pointed out [11], and Fateev and Wiegmann proved [12], using the Bethe ansatz method, that the spin of the system of the s-d model equals $S - 1/2$ in the ground state. The electrons interacting with the impurity in the s-wave can be considered as an one dimensional system. The total spin of the electrons, in the ground state, according to a theorem of Lieb and Mattis [13], takes the lowest possible value. If the number of electrons is odd, the total spin of the electrons (not including impurity spin) is equal to $1/2$, which coupled with the impurity spin leads to the total spin $S - 1/2$. The wave function of the system can be written as

$$\Psi = \psi_{-1/2} \chi_S + \psi_{1/2} \chi_{S-1},$$

where $\chi_S$ is the spin wave function of the impurity, and $M$ is the $z$ component of the spin of the impurity; $\psi_m$ is the wave function of electrons, and $m$ is the $z$ component of the total spin of electrons. The electrons away from the impurity are unpolarized, however, the localized electrons are polarized. So that $m$ is due to localized electrons. The numbers of the localized electrons in $\Psi$ satisfy conditions [9]:

$$n_{m}^{(1/2)} - 1 = n_{m}^{(1/2)} - 1,$$

where $n_{m}^{(1/2)}$ is the number of the localized electrons with spin up (down) in $\psi_m$. Condition (3) is the consequence of Anderson’s orthogonality theorem [14] and [9]. These conditions can be understood as follows. In the spin flip scattering, $\psi_{-1/2} \chi_S$ is transformed to $\psi_{1/2} \chi_{S-1}$, or vice versa, in other words, $\psi_{-1/2} \chi_S$ and $\psi_{1/2} \chi_{S-1}$ are connected by the s-d exchange interaction. The matrix element of the interaction Hamiltonian between $\psi_{-1/2} \chi_S$ and $\psi_{1/2} \chi_{S-1}$ nonvanished yields condition (3).

Now, let a uniform magnetic field $H$ in $-\hat{z}$ direction be switched on. Of course, the electron wave functions $\psi_{\pm 1/2}$ will vary and deviate from their original forms, and the $z$-components of the spins of the electron system will deviate
from $\pm \frac{1}{2}$, however, for convenience, we still denote them as $\psi_{\pm 1/2}$. Thus the subscripts $\pm \frac{1}{2}$ of $\psi_{\pm 1/2}$ do not indicate the z-components of the spin of the electron system to be $\pm \frac{1}{2}$ if $H \neq 0$. Furthermore, we assume that there is no components with $\chi_{M < S - 1}$ being generated as $H \neq 0$, because smaller $M$ is corresponding to higher Zeeman energy. So that we still have (2) and (3). Besides, we have charge neutrality condition:

$$
(n_{\uparrow}^{(-1/2)} + n_{\downarrow}^{(-1/2)})P_S + (n_{\uparrow}^{(1/2)} + n_{\downarrow}^{(1/2)})P_{S-1} = 0,
$$

where $P_S = \left| \langle \psi_{-1/2} | \psi_{-1/2} \rangle \right|^2$ and $P_{S-1} = \left| \langle \psi_{1/2} | \psi_{1/2} \rangle \right|^2$ are the probability of the system in states $\psi_{-1/2}\chi_S$ and $\psi_{1/2}\chi_{S-1}$, respectively. The wave functions $\Psi$ and $\chi_M$ have been normalized to unity, thus $P_S + P_{S-1} = 1$. The charge neutrality condition (4) can be justified by an inspection of the Bethe wave function [15] and [16]. The Bethe wave function shows that the number of the conduction electrons equals the total number of electrons, which implies that the total charge of the localized electrons vanishes.

It is evident that

$$
SP_S + (S - 1)P_{S-1} = \langle S^z \rangle
$$

and

$$
\frac{1}{2}(n_{\uparrow}^{(-1/2)} - n_{\downarrow}^{(-1/2)})P_S + \frac{1}{2}(n_{\uparrow}^{(1/2)} - n_{\downarrow}^{(1/2)})P_{S-1} = \langle S_z \rangle,
$$

where $\langle S^z \rangle$ ($\langle S_z \rangle$) is the expectation value of the z-component of the spin for the impurity (localized electrons) in the ground state.

Eqs. (3) and (4) lead to

$$
n_{\uparrow}^{(-1/2)} = -n_{\downarrow}^{(-1/2)}, \quad n_{\uparrow}^{(1/2)} = -n_{\downarrow}^{(1/2)}.
$$

Let us denote the z-component of localized spin as $M_i \equiv \langle S^z_i \rangle + \langle S^z_e \rangle$. Eqs. (5) - (7) and (3) lead to

$$
M_i = n_{\uparrow}^{(-1/2)} + S,
$$

and then

$$
n_{\uparrow}^{(-1/2)} = -n_{\downarrow}^{(-1/2)} = M_i - S,
$$

$$
n_{\uparrow}^{(1/2)} = -n_{\downarrow}^{(1/2)} = M_i - S + 1.
$$

From the Friedel sum rule [9,17] we immediately obtain the scattering phase shifts of the s-wave at the Fermi level:

$$
\delta^{(-1/2)}(\varepsilon_F) = -\delta^{(-1/2)}(\varepsilon_F) = \pi(M_i - S),
$$

$$
\delta^{(1/2)}(\varepsilon_F) = -\delta^{(1/2)}(\varepsilon_F) = \pi(M_i - S + 1),
$$

where $\delta^{(m)}(\varepsilon_F)$ is the scattering phase shift of the electron in state $\psi_m$ with z-component of spin $\sigma$. 

3
From (10) we obtain the impurity magnetoresistance:

\[ R(H) = R_0 \sin^2(\pi M_i), \quad S = \text{integer}, \]  

(11)

and

\[ R(H) = R_0 \cos^2(\pi M_i), \quad S = \text{half-integer}, \]  

(12)

where \( R_0 = R(H = 0) \) (remember \( M_i(H = 0) = S - 1/2 \)). When \( S = 1/2, \) (12) coincides with those obtained in [1]-[3] with \( M_i \) replaced by an approximate expression. The same expression of (12) for \( S = 1/2 \) was also given by [4].

3. Comparison with experimental data for \( S = 1/2 \)

We compare the theoretical result with experimental data in Fig.1. The solid curve for magnetoresistance \( R(H) \) versus \( H \) for \( S = 1/2 \) is obtained from (12). The experimental data for the magnetoresistance of \((\text{La,Ce})\text{Al}_2\) are taken from [8].

The dashed curve is obtained from (12), but takes the magnetization \( M^i \) from (9.25) of [15] of Andrei et al., and it is the same curve shown by Schlottmann in [5]. Fig.2 gives the magnetoresistance as a function of the magnetic field for impurities \( S = 1/2, 1, 3/2 \) obtained from (11) and (12). To compute \( R(H) \) (except those for the dashed curve in Fig.1) we have used the exact expression of \( M_i \) obtained by the Bethe ansatz method as follows,

\[ M_i(g\mu_B H) > 2k_B T_H = S - \frac{1}{2\pi^{3/2}} \int_0^\infty d\omega \frac{\sin(2\pi \omega S)}{\omega} \Gamma(1/2 + \omega) \left(\frac{\omega}{e}\right)^{-\omega} \times \exp[-2\omega \ln\left(\frac{g\mu_B H}{2k_B T_H}\right)] \]  

(13)

\[ M_i(g\mu_B H) < 2k_B T_H = S - 1/2 \]

\[ + \frac{1}{2\pi^{3/2}} \mathcal{P} \int_0^\infty d\omega \frac{\exp(2\omega \ln \frac{g\mu_B H}{2k_B T_H})}{\omega} \Gamma(1/2 - \omega) \left(\frac{\omega}{e}\right)^\omega \sin[2\pi(S - 1/2)\omega] \]

\[ + \sum_{n=0} \frac{(-1)^n \left(\frac{g\mu_B H}{2k_B T_H}\right)^{2n+1}}{2\sqrt{n!(n + 1/2)}} \left(\frac{n + 1/2}{e}\right)^{n+1/2} \cos[2\pi(S - 1/2)(n + 1/2)] \]

(14)

where \( T_H = \frac{2N}{L} \sqrt{\frac{\pi}{2\epsilon}} e^{-\pi/g'} \) with \( g' = \frac{1}{S+1/2} \tan[(S + 1/2)J/2]. \) (This \( T_H \equiv (T_H)_{\text{Wiegmann}} \) is defined as that in [16], not as \( T_H \equiv (T_H)_{\text{Andrei}} \) in [15]. The relation between them is \((T_H)_{\text{Wiegmann}} = \sqrt{S}(T_H)_{\text{Andrei}} \) for \( J << 1. \) \( N \) is the number of electrons, \( L \) is the length of the system, \( \mu_B \) is the Bohr magneton, and \( g \) is the Landé g-factor.

We have to make some remarks.

1. Eqs. (13) and (14) are essentially the same as (31) and (33) of [12] (where \( g = 2, \mu_B = 1, k_B = 1 \)), respectively, but with corrections: (a) in (33) of [12] \( \int_0^\infty d\omega \ldots \) is replaced by the principal-value integral \( \mathcal{P} \int_0^\infty d\omega \ldots , \) and \( \sum_{n=0}^\infty \ldots \) \( \ldots \) is replaced by \( \frac{1}{2} \sum_{n=0}^\infty \ldots , \) (b) in (33) of [12] the integrand multiplies a factor \( \sin[2\pi(S - 1/2)\omega], \) (c) in (31) and (33) of [12] \( T_K \) is replaced by \( T_H \). Corrections (b) and (c) have already been done by [16].
2. To derive (13) and (14), the Pauli susceptibility is assumed to be \( \chi = L/2\pi \) (for \( \mu_B = 1 \), \( g = 2 \)) in one dimensional space which corresponds to take the coupling constant \( J = 0^+ \). This value of \( \chi \) coincides with that adopted by Tsvelick and Wiegmann [16], but different from that adopted by Andrei et al. [15]. Andrei et al. assumed the value of \( \chi \) corresponding to \( J = 0 \). Since the density of states at the Fermi level for \( J = 0 \) is two times for \( J = 0^+ \) in the Bethe ansatz method, the Pauli susceptibility adopted by Andrei et al. equals \( \chi = L/\pi \). In our opinion, it is appropriate to take \( J = 0^+ \). If one assumes \( J = 0 \), as Andrei et al., the factor \( \frac{\mu B H}{g_k B T_h} \) in (13) and (14) should be replaced by \( \frac{\mu B H}{g_k B T_h} \).

3. A similar comparison between the experimental magnetoresistance and the theoretical result of Andrei for \( S = 1/2 \) [4] has been done by Schlottmann [5]. However, what we do here is different form [5]. In [5], (a) the experimental electric resistivity is less than those obtained by Felsch et al. [8] about 0.6/\( \mu \) cm although [5] referred to [8], (b) to compute \( M \), Schlottmann [5] used the result of [15], where the Pauli susceptibility \( \chi \) corresponding to \( J = 0 \). With corrections on these two points, we see that the theoretical curve for \( S = 1/2 \) fits the experimental data well except at \( H = 50 \) Oe.

4. Conclusion

The magnetoresistance of s-d model with arbitrary impurity spin in the ground state is obtained by combining the Yosida-Yoshimori method and results from the Bethe ansatz. The comparison of the magnetoresistance of the s-d model for \( S = 1/2 \) in the ground state with experimental data is re-examined. We have shown that one should use (13)-(14) to calculate the magnetoresistance to fit the experimental data. As shown in Fig. 1, the solid curve is closer to the experimental data than the older result (the dashed curve).

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References

[1] H. Ishii, Prog. Theor. Phys. 43, 578 (1970).
[2] D. R. Hamann, Phys. Rev. B2, 1373 (1970).
[3] K. Yosida and A. Yoshimori, in Magnetism, Vol. 5, edited by G. Rado and H. Suhl (New York, Academic Press 1973).
[4] N. Andrei, Phys. Lett. 87A, 299 (1982). See also [14].
[5] P. Schlottmann, Phys. Rev. B35, 5279 (1987).
[6] P. Schlottmann, Phys. Rep. 181, 4 (1989).
[7] A. C. Hewson, The Kondo Problem to Heavy Fermions (Cambridge, Cambridge Univ. Press 1996).
[8] W. Felsch and K. Winzer, Solid State Commun. 13, 569 (1973).
[9] K. Yosida, Theory of Magnetism (Springer, Berlin 1996).
[10] V. A. Fateev and P. B. Wiegmann, Phys. Lett. 81 A, 179 (1981); Phys. Rev. Lett. 46, 1595 (1981). See also A. M. Tsvelick and P. B. Wiegmann, Adv. Phys. 32, 453 (1983), and H. Furuya and J. H. Lowenstein, Phys. Rev. B 25, 5935 (1982).
[11] D. Mattis, Phys. Rev. Lett. 19, 1478 (1967).
Figure Captions

Fig.1 Magnetoresistance of (La, Ce)Al$_2$. The experimental data are taken from [8]. The magnetoresistance $R(H)$ corresponding to $S = 1/2$ shown by the solid curve is obtained by using (12) - (14) with $T_H = \frac{1}{4\pi} \sqrt{\frac{2\pi}{eT} T_K}$, and the Wilson number $W = 1.290265$ [15]. The Kondo temperature $T_K = 0.20K$ and $g = 10/7$ are the same ones used by Rajan et al. [18]. The dashed curve is obtained by using $\mathcal{M}^c$ of (9.25) in [15] of Andrei et al., who assumed the Pauli susceptibility corresponding to $J = 0$, and it is just the curve of Schlottmann [5].

Fig.2 The magnetoresistance as a function of the magnetic field obtained from (11)-(14) for impurities $S = 1/2, 1, 3/2$. The parameters are the same as those in Fig.1.
Fig. 1 Ding et al
Fig. 2 Ding et al