Unconventional One-Magnon Scattering Resistivity in Half-Metals

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(Received )

Low-temperature resistivity of half-metals is investigated. To date it has been discussed that the one-magnon scattering process in half-metals is irrelevant for low-temperature resistivity, due to the fully spin-polarized electronic structure at the ground state. If one takes into account the non-rigid-band behavior of the minority band due to spin fluctuations at finite temperatures, however, the unconventional one-magnon scattering process is shown to be most relevant and gives $T^3$ dependence in resistivity. This behavior may be used as a crucial test in the search for half-metallic materials which are potentially important for applications. Comparison with resistivity data of La$_{1-x}$Sr$_x$MnO$_3$ as candidates for half-metals shows good agreement.

KEYWORDS: half-metal, ferromagnetic metal, one-magnon resistivity, colossal magnetoresistance manganites

Since Zener introduced the double exchange (DE) model as a model for perovskite manganites $\text{AMnO}_3$, intensive studies have been performed. Nevertheless, spin fluctuation effects beyond the mean-field picture have not yet been fully clarified. Spin fluctuations strongly influence the structure of the conduction electron band in the DE model. Therefore, many-body treatments with respect to spin fluctuations are important. One example of the mean-field treatment giving an inaccurate result is that it substantially overestimates the Curie temperature $T_c$. Using realistic parameters for La$_{1-x}$Sr$_x$MnO$_3$, Millis et al. demonstrated that the mean-field treatment of the DE model gives $T_c = 1000$ K $\sim 3000$ K, which is much larger than the experimental values $T_c = 300$ K $\sim 400$ K at $0.2 < x < 0.5$, and concluded that the DE model alone cannot explain La$_{1-x}$Sr$_x$MnO$_3$. However, by considering thermal spin fluctuations at $T \sim T_c$, which reduce electronic hoppings, the model reproduces experimental $T_c$.

Resistivity is also strongly influenced by spin fluctuations. Kubo and Ohata investigated the resistivity of the DE model. The ground state of this model is perfectly spin-polarized, and is now called half-metallic. Based on a rigid-band picture, they have proposed that two-magnon processes which give $\rho \propto T^4$ are relevant for the low-temperature resistivity. In this Letter, however, we demonstrate that a different scattering process creates $\rho \propto T^3$ in half-metals. This process appears only by considering spin fluctuations beyond the rigid-band approximation.

Half-metals interest us from the viewpoint of fabricating a tunneling magnetoresistance junction, since the perfect spin polarization of conduction electrons is important for the sensitivity of devices. Indeed, the origin of low-field magnetoresistance in polycrystal and tri-layer junctions of manganites is considered to be the spin-dependent tunneling at half-metallic junctions. We also note that an exotic type of superconductivity in half-metals has been predicted. In order to conduct a material search for half-metals, a unique $T$-dependence in resistivity might play an important role as a crucial test.

The magnetic scattering of quasiparticles is one of the origins of resistivity in magnetic metals. In conventional itinerant weak ferromagnets, the one-magnon scattering (1MS) process illustrated in Fig. 1, is one of the origins of resistivity in the form $\rho \propto T^2$. The existence of coherent quasiparticles for both majority- and minority-spin bands is essential for the conventional 1MS process, since the process involves spin-flipping vertices and a propagator of the minority band at the Fermi level.

On the other hand, half-metals belong to a different class of itinerant ferromagnets. Conduction electrons are perfectly spin-polarized, and the Fermi surface is absent in the minority-spin band. In Fig. 2(a) we illustrate the density of states (DOS) for a large Hund’s coupling ($J_H$) region of the DE model as a canonical example. Kubo and Ohata stated that the 1MS is forbidden in the DE model due to its half-metallic ground state.

However, spin fluctuations at a finite temperature create modifications of the electronic band structure. In
Fig. 1. 1MS self-energy diagram for the majority band. The solid line and the dashed curve represent electron and magnon Green’s functions, respectively.

Fig. 2(b) we illustrate the DOS at $0 < T < T_c$. The DOS has been calculated by the dynamical mean-field (DMF) theory which takes local spin fluctuations into account, and also by the Monte Carlo method which treats spin fluctuations on a finite size cluster in an controlled manner. At a finite temperature, spin fluctuations induce a minority band. Once the thermally activated minority band is created and occupied, a 1MS is allowed. This 1MS is unconventional in the sense that it is absent at the ground state and is strongly affected by the spin fluctuation.

Based on such a non-rigid-band picture, we calculate the resistivity of half-metals in three dimensions. We consider a magnon-electron interaction in the form

$$H_{\text{int}} = \frac{g}{\sqrt{N}} \sum_{qk} \left( a_k^\dagger c_{k+q}^\dagger c_{k+q} + a_k^\dagger c_{k}^\dagger c_{k+q}^\dagger c_{k+q} \right),$$

where $c^\dagger$ and $a^\dagger$ are the creation operators for electrons and magnons, respectively. We define the quantization axis in such a way that a magnon carries $S_z = -1$. For the DE model, the electron-magnon coupling constant is given by $g = J_H/\sqrt{N}$ where $J_H$ gives the Hund’s coupling between conduction electrons and localized spins. Therefore, a perturbational approach based on the linear magnon approximation is well defined, at least in the limit $S \rightarrow \infty$, where $J_H$ is kept constant, and presumably gives qualitatively correct results at low temperatures where spin fluctuations are sufficiently small.

Since conductivity is governed by the majority carriers, the self-energy for the majority spin electrons $\Sigma^\uparrow$ determines the low-temperature resistivity. A 1MS self-energy, illustrated in Fig. 1, is given in the form

$$\Sigma^\uparrow(k, \omega) = \frac{g^2}{N} \sum_q \int \frac{d\omega'}{2\pi} G_\downarrow(k+q, \omega+\omega') D(q, \omega'),$$

where $G_\downarrow$ and $D$ are Green’s functions for minority-spin electrons and magnons, respectively. Note the direction of the magnon propagator. The 1MS for a majority band electron occurs only when it absorbs a magnon carrying $S_z = -1$. The intermediate state involves a propagator of the preoccupied minority band. Thus, the 1MS self-energy strongly depends on spin fluctuations and diminishes at $T \rightarrow 0$.

Let us assume that Green’s function for the minority band obtained by the DMF is also valid in three-dimensional systems, which at small frequencies reads

$$G_\downarrow(k, \omega) \simeq \frac{z_\downarrow}{\omega - \zeta_\downarrow(k) - i\Gamma_\downarrow},$$

The quasiparticle renormalization factor scales as

$$z_\downarrow = \delta m/2,$$

where $\delta m = (M(0) - M(T))/M(0)$ is the reduction of the spin moment $M(T)$ scaled by its saturated value $M(0)$. Quasiparticle dispersion relation is denoted by $\zeta_\downarrow(k) = (W^* / W)\varepsilon_k - \mu$. Here, $\varepsilon_k$ is the dispersion relation of the majority band at $T = 0$, and $\mu$ is the chemical potential, while $W$ and $W^*$ are the quasiparticle bandwidth at $T = 0$ and finite $T$, respectively, which scales as $W^* / W \simeq \delta m / 2$. The inverse lifetime for the minority band due to spin-disorder localization is given by $\Gamma_\downarrow \sim W(1 - \delta m / 2)$.

At low temperatures where $\delta m \ll 1$, we have the incoherent limit for $G_\downarrow$, namely $|\zeta_\downarrow(k)| \ll \Gamma_\downarrow$. Then, the conventional 1MS calculation becomes invalid. The integration in eq. (2) is dominated by the pole in the magnon Green’s function. As a rough estimate, we have

$$\text{Im} \Sigma^\uparrow \sim \frac{z_\downarrow}{\Gamma_\downarrow} \frac{1}{N} \sum_{q,n} D(q, i\Omega_n) \propto z_\downarrow \langle n_{\text{mag}} \rangle,$$

where $\langle n_{\text{mag}} \rangle$ is the magnon occupation number per site.
which satisfies $\delta m = \langle n_{\text{mag}} \rangle / M(0)$. Therefore, the inverse lifetime of the majority spin carrier at the Fermi level $\Gamma_\uparrow = \mathcal{I}m \Sigma_\uparrow(k = k_F, \omega = 0)$ is proportional to the square of the spin fluctuation, $\Gamma_\uparrow \propto (\delta m)^2$. For three-dimensional magnons with the dispersion relation $\omega_q = D_n q^2$, where $D_n$ is the spin stiffness, we have $\langle n_{\text{mag}} \rangle \simeq 0.06(T/D_n)^{3/2}$. Using the Drude formula $\rho = (m^*/ne^2)\Gamma_\uparrow$, we obtain

$$\rho \propto (T/D_n)^3. \quad (6)$$

More formal expression for $\Sigma_\uparrow$ is obtained through the spectral representation as

$$\mathcal{I}m \Sigma_\uparrow(k, \omega - i\eta) = \frac{g^2}{N} \sum_q \int_{-\infty}^{\infty} d\omega' \left[ f(\omega + \omega') + n(\omega') \right]$$

$$\times \mathcal{I}m G_\downarrow(k + q, \omega + \omega' - i\eta) \mathcal{I}m D(q, \omega' - i\eta), \quad (7)$$

where $f(\omega)$ and $n(\omega)$ are Fermi and Bose distribution functions, respectively. The incoherent limit of eq. (3) gives $\mathcal{I}m G_\downarrow(k, \omega - i\eta) \simeq z_\downarrow/\Gamma_\downarrow$, and for the magnon Green’s function we use $\mathcal{I}m D(q, \omega - i\eta) = \pi\delta(\omega - \omega_q)$. Then, we obtain

$$\Gamma_\uparrow = g^2 z_\downarrow N \sum_q \left[ f(\omega_q) + n(\omega_q) \right] \sim g^2 z_\downarrow (n_{\text{mag}}). \quad (8)$$

Here, we use $f(\omega) \ll n(\omega)$ at small frequencies which mostly contributes to the integration.

We point out here that $T^3$ resistivity can be used as a probe to investigate whether a given compound is a half-metal. For example, if there exists a substantial overlap with other bands, it will create a conventional $T^2$ resistivity. Wang and Zhang calculated the case of a nearly half-metal where the slightly doped minority band is Anderson-localized below the mobility edge. They derived the resistivity $\rho \propto T^{2.5}$ at high temperatures which crosses over to $\rho \propto T^{1.5}$ at low temperatures.

Let us now compare the result with those of experiments. We investigate the resistivity data for $La_{1-x}Sr_xMnO_3$ as a candidate for a half-metal. It has previously been shown by various experiments that the spin polarization of the conduction electron is very large; large values of saturation moment $\sim 4\mu_B$ suggest that Mn ions are in high-spin states. Spin-dependent photoemission experiments as well as tunneling magneto-resistance measurements indicate the absence of the minority-spin quasiparticles at the Fermi level. Observation of magnon dispersion throughout the Brillouin zone supports the hypothesis that the low-energy Stoner continuum is absent due to large spin polarization. Nevertheless, since there exist overlaps of Mn $e_g$ orbitals and O $2p$ orbitals in the conduction band which might break down the perfect spin-polarization, it is important to determine whether these series of compounds are half-metals or not. Here, we examine whether they can be considered as perfectly spin-polarized half-metals, on the basis of the low-temperature resistivity measurements.

Low-temperature resistivity data for single crystals of $La_{1-x}Sr_xMnO_3$ are obtained from ref. The residual resistivity of the sample is $\rho_0 \leq 35\mu\Omega\text{cm}$ at $x = 0.4$ indicating the high quality of the sample. In Fig. 3, we show the conventional $T^2$-plot of the resistivity $\rho(T)$. In the high-temperature region, the resistivity data fit well in the form $\rho(T) = \rho_0 + AT^\alpha$ with $\alpha \simeq 2$, as has been commonly reported for metallic manganites.

However, in the low-temperature region below 20 K we see substantial deviation from the $T^2$-like behavior. The flattening of $\rho(T)$ is observed. Moreover, there exist discrepancies between $\rho_0 = \rho(T \to 0)$ and its counterpart by extrapolation from the high-temperature $T^2$ region, $\rho_0$. The reduction of the resistivity $\rho(T) < \rho_0$ indicates that $\rho(T)$ is not understood by Matthiessen’s rule, i.e., $\rho(T)$ at $T \gtrsim 20$ K is not explained by the simple sum of the residual scattering and the Fermi-liquid-type scattering at $T \to 0$. Namely, this indicates that not only the quasiparticle lifetime but also the nature of the conduction channel itself might possibly make a crossover at $T \sim 20$ K.
Let us now restrict ourselves to the low-temperature region below the crossover, and examine the 1MS results. In Fig. 4 we show a $T^3$-plot of the resistivity $\rho(T)$. The data at $T \lesssim 30$ K is well reproduced by the unconventional 1MS contribution $\rho(T) = \rho_0 + A_3 T^3$. We also investigate the coefficient of the $T^3$ term as a crucial test. From eq. (6) we expect the scaling relation $A_3 \propto D_x^{-3}$. Unfortunately, the values of $D_x$ have been measured for only a few limited concentrations thus far, so a direct comparison cannot be carried out. Instead, we assume a scaling relating $D_x \propto x$, which is experimentally observed in La$_{1-x}$Sr$_x$MnO$_3$ at $0.15 \lesssim x \lesssim 0.3$. In Fig. 5 we plot the coefficient of the $T^3$ term as a function of doping, and we roughly see $A_3 \propto x^{-3}$. The deviation from the fit at $x = 0.4$ can be understood by the saturation of $D_x$ as a function of $x$, since we experimentally see that at $x \sim 0.4$ the increase of $T_c$ by increasing $x$ saturates and $D_x$ roughly scales as $T_c$. In this analysis we assumed that the carrier number $n$ and the effective mass $m^*$ do not change substantially upon doping in the metallic region, based on the Hall coefficient and specific-heat measurements.

The $T^3$ behavior as well as the concentration dependence of its coefficient shows consistent theoretical and experimental results. Another possible test is to measure the resistivity under high magnetic fields which suppress $\delta m$. Resistivity due to the unconventional 1MS should scale as $\rho(T, H) = \rho_0 \propto (\delta m(T, H))^2$.

Thus, the low-temperature $T^3$ behavior in the resistivity of (La,Sr)MnO$_3$ is direct evidence of their half-metallic nature. Similar behaviors have been reported for various compositions of doped manganites in the ferromagnetic metal regime. Crossovers from $T^2$-like behavior to a flatter temperature dependence in the low-temperature region is widely seen. Recently, resistivity data for narrow bandwidth compounds including (Nd,Sr)MnO$_3$ and (Sm,Sr)MnO$_3$ were shown to fit well with $T^3$ at low temperatures. We also note that a similar flattening in the low-temperature resistivity is also observed in CrO$_2$, which is considered to be another half-metallic system.

Let us discuss the applicability of the DMF. In eq. (3), we see that $G_{\uparrow}$ has nonzero $\Gamma_1$ for $k = k_F, \omega = 0$ in the limit $T \to 0$. This behavior seems to be an artifact of the DMF approximation, which should be recovered by taking into account proper vertex corrections as a magnon-drag phenomenon. For the majority-band self-energy, however, this recovery of coherence is not exhibited at low temperatures. The minority-band Green’s function should exhibit an incoherent behavior in the high-frequency region $|\omega| \gtrsim W^*$, irrespective of the vertex correction. The majority-band self-energy in eq. (5) is determined by the minority-band structure in the frequency range $|\omega| \lesssim T$. Since $W^* \propto T^{3/2}$, contributions from the incoherent part of $G_{\downarrow}$ become dominant in eq. (3) when $W^* \ll T$. Incoherent treatments for the minority-band Green’s function appear to be valid at low temperatures.

Once an incoherent minority band with the weight $z_{\downarrow} \propto \delta m$ is created, we have $\rho \propto T^3$. Note that localization effects as well as strong electron-electron inter-
actions enhance the incoherence of the minority band, which enlarge the $T^3$ scaling region. The crossover temperature $T^*$ is roughly estimated by

$$T^* \sim W^* \simeq (0.06W/2M(0)) \cdot (T^*/D_s)^{3/2}. \quad (9)$$

Using the parameters for (La,Sr)MnO$_3$, $W \sim 1$eV, $D_s \sim 10$ meV and $M(0) \sim 2$, we obtain $T^* \sim 50$ K, which is consistent with the actual crossover temperature in experiments, $T_{exp} \sim 30$ K, where deviations from the $T^3$ behavior emerge. Above $T^*$, the minority band quasiparticles gain coherence since $W^* > T$. The change in the electronic structure causes a deviation from the $T^3$ behavior. Electronic properties at $T > T^*$, particularly the minority-band Green’s function structure and its influences to the 1MS, remain for future study in order to explain the $T^2$-like resistivity in experiments.

In the low-temperature region of manganites $T < T_c$, where spin moments are considered to be almost saturated, the roles of orbital degeneracies have been emphasized, which should contribute to the Fermi-liquid-type $T^2$ resistivity down to $T \to 0$. However, the $T^3$ behavior of the resistivity at $T \ll T^*$ in Fig. 4 indicates that the $T^2$ contributions are negligible. Hence, concerning this temperature region of measurement, $T \ll T^* \ll T_c$, the spin fluctuation scattering is much stronger than other scattering mechanisms.

To summarize, the low-temperature resistivity of half-metals is investigated. On the basis of the unconventional 1MS contribution, we obtain $T^3$ behavior below the crossover temperature $T^*$. We conclude that this is a unique character of half-metals, and may be used as a crucial test to make the distinction from conventional itinerant ferromagnets. Comparison with experimental data for a possible half-metal (La,Sr)MnO$_3$ reveals good agreement. The author thanks A. Asamitsu and Y. Tokura for providing the data in ref. [18] as well as for useful comments. He is also grateful M. Salamon, M. Jaime, A. J. Millis, A. Gupta, Y. Moritomo and G. M. Zhao for valuable discussions.

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