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Phenomenological theory of the resistivity of MnSi above the critical pressure

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Abstract

The electrical resistivity of a metal close to a weakly first-order paramagnetic-to-ferromagnetic transition at $T = 0$ is determined assuming that droplets of magnetic order remain in the paramagnetic state. Using an elementary model of spin-diffusion to describe the spin dynamics, it is found that, at low temperatures, the resistivity ρ varies as $\rho = \rho_0 + aT^{3/2}$. The temperature-dependent term occurs because of the scattering of electrons by low-frequency spin fluctuations propagating normal to the surface of the ferromagnetic regions. The temperature dependence is in agreement with recent measurements made on MnSi at pressures above the critical pressure. The pressure dependence of the model prediction for a is also found to be in qualitative agreement with the variation observed experimentally above the critical pressure.

When the itinerant ferromagnet MnSi is studied under applied pressures large enough to suppress ferromagnetism at $T = 0$ (i.e. $P > P_C$), an unusual paramagnetic phase is seen. This was discovered through recent measurements [1] of the electrical resistivity ρ in this system, which showed that $\rho = \rho_0 + \rho(T)$, where $\rho(T) = aT^{3/2}$ over temperatures ranging from 50 mK to 6 K, and over a pressure range extending from the critical pressure P_C to more than $2P_C$. The measured resistivity contradicts Fermi-liquid theory, which predicts that $\rho(T)$ should be proportional to T^2 at low T. Conventional theory of ferromagnetic metals [2–6] allows for violations of Fermi-liquid behaviour at finite temperatures near a phase transition, but does not predict well-defined $T^{3/2}$ behaviour, and thus cannot account for the data. The breakdown of Fermi-liquid theory was particularly surprising given that the $T = 0$ transition with pressure is first order, so that critical fluctuations are not expected to be significant even close to P_C. The finding has stimulated a renewal of interest in this material [7, 10–13].

In an attempt to explain the T-dependence of the electrical resistivity, the authors of [1] suggested that droplets of ferromagnetic order might remain in the system at pressures well above P_C, and that spin fluctuations associated with these droplets could provide a scattering mechanism that leads to non-Fermi-liquid behaviour. They pointed out that this scenario is plausible in MnSi, since the phase transition is only weakly first order and thus the free-energy cost of ferromagnetic regions in the paramagnetic state should be relatively small. Recent

NMR measurements [7] made on MnSi above P_C at low temperature have also indicated the presence of spatial inhomogeneity in the electronic spin system, which may be interpreted as support for the droplet picture.

In this paper I investigate this picture using a very simple approach. I assume that such ferromagnetic regions exist at $P > P_C$ and determine their expected effect on the low-frequency spin dynamics using a phenomenological spin-diffusion model. I then calculate the electrical resistivity that results when electrons are scattered mainly by the long-wavelength spin fluctuations associated with the relaxation of magnetic order in the droplets.

As the main result of this paper, I find that the observed temperature dependence of the resistivity, $\rho(T) = aT^{3/2}$, emerges as low-temperature behaviour of the model. (The constant ρ_0 term is attributed to scattering from impurities and will not be discussed.) The most intriguing aspect of the MnSi resistivity data, the persistence of the $T^{3/2}$-dependence down to millikelvin temperatures, is thus captured. I compare the predicted pressure dependence of the coefficient a with the observed variation and find qualitative agreement.

The presentation of this paper will be given as follows. I shall begin by deriving an effective dynamic spin susceptibility assuming that the low-frequency response is dominated by the droplets. I calculate the imaginary part of the electron self-energy to lowest order (with the derived dynamical susceptibility playing the role analogous to the phonon propagator in the corresponding lowest-order electron–phonon diagram) and insert the result into a Boltzmann expression for the current in order to obtain $\rho(T)$. After this I will discuss some of the assumptions used in the model before concluding.

The rate of relaxation of the spin density near a region of ferromagnetic order is expected to occur via diffusion of spins through the surface of the region [8, 9]. Taking $\psi(\mathbf{r}, t)$ to be the expectation value of the $\hat{\mathbf{z}}$-component spin-density, I assume that the relaxation may be described using a diffusion equation:

$$\frac{\partial}{\partial t}\psi(\mathbf{r}, t) = \tilde{D}\frac{\partial^2}{\partial r_n^2}[\psi(\mathbf{r}, t) - \psi_0(\mathbf{r}, t)] \tag{1}$$

where $\tilde{D}$ is a diffusion constant, r_n is the component normal to the surface and $\psi_0(\mathbf{r}, t)$ is the corresponding equilibrium spin density in the presence of a weak time- and space-dependent magnetic field parallel to $\hat{\mathbf{z}}$ with magnitude $h(\mathbf{r}, t)$. Using mean field theory, the equilibrium part is obtained as

$$\psi_0(\mathbf{r}, t) = \chi_0[h(\mathbf{r}, t) + (\alpha + c\nabla^2)\psi(\mathbf{r}, t)] \tag{2}$$

where χ_0 is the spin susceptibility of a non-interacting system and α, c are constants. Assuming a plane-wave form for both the applied field and the spin density, the dynamic spin susceptibility is obtained[1] from equations (1) and (2) as

$$\chi^{-1}(\mathbf{q}, \omega) = \chi_{\mathbf{q}}^{-1}[1 - \mathrm{i}\omega/\Gamma_{\mathbf{q}}], \tag{3}$$

where

$$\Gamma_{\mathbf{q}} = Dq_n^2\chi_{\mathbf{q}}^{-1}, \tag{4}$$

q_n is the component of the wavevector in the direction normal to the droplet surface and $D = \chi_0\tilde{D}$ defines a new diffusion constant. The static susceptibility may be written in terms of a static correlation length ξ (and the constant α thus eliminated) as

$$\chi_{\mathbf{q}}^{-1} = \chi^{-1} + cq^2 \qquad \text{with } \chi^{-1} = c\xi^{-2}. \tag{5}$$

Some spatial dependence corresponding to the distribution of droplets is contained implicitly in equation (4) since $\hat{\mathbf{q}}_n$ must be interpreted as the direction normal to the nearest

[1] M B Walker suggested a similar form for $\chi(\mathbf{q}, \omega)$ in private communication with the author.

droplet surface. When I calculate the electrical resistivity, I simulate an average over different spatial configurations of the droplets by averaging over $\hat{\mathbf{q}}_n$. In addition, a minimum cutoff of q_n will be imposed, such that $q_n > q_0$, where q_0^{-1} is regarded as the characteristic length scale of the fluctuations[2]. Finally, the number density of the droplets will be incorporated into an electron-spin fluctuation coupling parameter J^2 that is introduced below. It will be assumed in this paper that, at sufficiently low-T in the vicinity of the pressure-induced critical point, ξ, q_0 and J^2 depend on pressure but are independent of temperature.

Lonzarich and Taillefer [5] (henceforth LT) derived an expression for the dynamic susceptibility of a nearly ferromagnetic metal starting from a simple microscopic model. (Although similar expressions can be found in other works, reference [5] is convenient for present purposes since LT made a detailed analysis of MnSi data.) Their result is of the same form as equations (3) and (5), but instead of equation (4) they used $\Gamma_{\mathbf{q}} = \gamma q \chi_{\mathbf{q}}^{-1}$, where γ is a constant, which describes Landau damping of spin fluctuations. They found that the low-pressure magnetic properties of MnSi can be explained using their model with values for γ and c obtained from neutron scattering measurements. I shall make use of the correspondence between the current model and that of LT. The values of c and γ that LT obtained will be assumed to be approximately correct over the high-pressure range considered here, and will thus be used, along with the measured homogenous susceptibility $\chi(P > P_C)$, for numerical estimates. The model for the electrical resistivity that I study depends on the remaining parameters D and q_0, as well as the factor J^2 that contributes to the overall scale.

By adopting the phenomenological expression, equation (4), to describe diffusive spin relaxation occurring in the high-pressure paramagnetic state, I find below that the anomalous $T^{3/2}$ term in the resistivity is naturally explained. Since this diffusive mechanism is not expected to be important within the ordered state, it is reasonable to expect an abrupt change in the qualitative behaviour of the resistivity to occur at the first-order phase transition, as is observed [1] ($\rho(T) \propto T^2$ at low T in the ferromagnetic state of MnSi). Only the paramagnetic state, with zero applied magnetic field, will be considered in this paper.

The imaginary part of the retarded electron self-energy, calculated to lowest order in the interaction with the spin fluctuations described above, is

$$\mathrm{Im}\Sigma_R(\mathbf{p},\omega) = -J^2 n_0 \frac{V}{(2\pi)^3}\int \mathrm{d}\epsilon\, \epsilon(f(\epsilon+\omega)+n(\epsilon))\int \frac{\mathrm{d}S_{\mathbf{k}}}{|v_{\mathbf{k}}|}\frac{\chi_{\mathbf{k}-\mathbf{p}}\Gamma_{\mathbf{k}-\mathbf{p}}}{\epsilon^2+\Gamma_{\mathbf{k}-\mathbf{p}}^2}, \tag{6}$$

where I have introduced the (pressure-dependent) coupling energy J^2 and where n_0 is the density of states, $\mathbf{v}_{\mathbf{k}}$ is the Fermi velocity, V is the sample volume, $f(\epsilon)$, $n(\epsilon)$ are Fermi, Bose functions and the second integral is over the Fermi surface. I will not go beyond this lowest-order calculation of the self-energy. The spin-susceptibility in equation (6) is an effective expression and will thus not be renormalized (the effect of Landau damping will be discussed briefly below) while imaginary self-energy corrections to the electron propagator can be ignored at sufficiently low T since it is determined below that the scattering rate vanishes at least as quickly as $T^{3/2}$.

For simplicity, I consider a single isotropic band. The average over $\hat{\mathbf{q}}_n$, denoted by large angular brackets in equation (7), gives the following:

$$\left\langle \int \frac{\mathrm{d}S_{\mathbf{k}}}{|v_{\mathbf{k}}|}\frac{\chi_{\mathbf{k}-\mathbf{p}}\Gamma_{\mathbf{k}-\mathbf{p}}}{\epsilon^2+\Gamma_{\mathbf{k}-\mathbf{p}}^2}\right\rangle = \frac{\pi}{v_f\sqrt{D\epsilon}}\int_{q_0}^{q_c}\mathrm{d}q\, \chi_{\mathbf{q}}^{3/2}\kappa_{\mathbf{q}}(\epsilon), \tag{7}$$

[2] It is assumed that ferromagnetic regions exist, but left undetermined whether the regions are purely dynamic or static regions with a dynamic surface [7]. The length scale q_0^{-1} can be regarded as the size of the droplet in the former case and the thickness of the surface in the latter. Also, the model may be applicable (at least for the scattering contribution of longitudinal spin fluctuations) if the ferromagnetic volume fraction is significant as long as the measured χ, which contains information about the pressure dependence of the ferromagnetic volume fraction, is used.

where

$$\kappa_{\mathbf{q}}(\epsilon) = \int_{x_1}^{x_2} \mathrm{d}x \, \tan^{1/2}(x) \tag{8}$$

and

$$x_1 = \arctan\left(\frac{Dq_0^2\chi_{\mathbf{q}}^{-1}}{\epsilon}\right), \qquad x_2 = \arctan\left(\frac{Dq^2\chi_{\mathbf{q}}^{-1}}{\epsilon}\right). \tag{9}$$

An upper limit of the q-integral q_c has been introduced. The Fermi surface imposes a limit $q < 2k_f$, but the model for the susceptibility is expected to break down for values of q that are considerably smaller. I shall assume that q_c is some reasonable fraction of k_f.

The value of ξ is estimated [1] to be 6 Å for MnSi at pressures just above P_C and to be slightly smaller at $2P_C$ (this is determined using the value $c = 2.1 \times 10^4$ Å^2 obtained by LT and the measured static homogenous susceptibility $\chi = \xi^2/c$ from [14]). It is thus expected that $q_c \leqslant \xi^{-1}$, which means that $\chi_{\mathbf{q}}$ can be well approximated by χ over the pressure range of interest.

The low-energy limit is defined by $\epsilon \ll k_B T_0$, where

$$k_B T_0 = Dq_0^2\chi^{-1} \tag{10}$$

is the crossover temperature. In this limit, $\kappa_{\mathbf{q}}(\epsilon) = \sqrt{\epsilon/(Dq_0^2\chi^{-1})}$, and thus the Fermi-surface integral is independent of energy. The electron scattering rate τ^{-1} is determined from equations (6) and (7) to be

$$\tau^{-1}(T) = -2\mathrm{Im}\Sigma(T) = K\frac{(k_B T)^2}{k_B T_0}, \tag{11}$$

where the dimensionless prefactor is given by

$$K = \frac{J^2 n_0^2 \pi^2}{4}\left(\frac{\chi q_c q_0}{k_f^2}\right). \tag{12}$$

The limit $k_B T \gg \omega$ has been taken to obtain the T-dependent scattering rate (the opposite limit gives the same result to within a factor of order unity with $k_B T$ replaced by ω).

The T^2 Fermi-liquid behaviour is retained as the low-T limit of the electron–electron scattering rate. From equation (10), the crossover temperature T_0 is proportional to $q_0^2\xi^{-2}$, so T_0 decreases as the square of the droplet size (see footnote 2) q_0^{-1}, and thus becomes low if the droplets become large while the static correlation length remains small. The correlation length ξ is only weakly pressure dependent above P_C (according to [1], it increases by less than a factor of two, reaching its maximum of 6 Å when the pressure is decreased from $2P_C$ to P_C). Naively, one expects that q_0^{-1} will decrease with increasing pressure above P_C. This would indicate an increase of T_0 with pressure, and thus a return to Fermi-liquid behaviour at sufficiently large pressure for any given temperature.

At energies above $k_B T_0$ and below[3] $k_B T_1 = Dq_c^2\chi^{-1}$, the q integral is dominated by $q \approx q_c$. Thus one takes $x_1 = 0$ and $x_2 = \pi/2$ so that equation (8) becomes $\kappa_{\mathbf{q}}(\epsilon) = \pi/\sqrt{2}$. The scattering rate is then found as

$$\tau^{-1}(T) = K\eta\frac{(k_B T)^{3/2}}{\sqrt{k_B T_0}}, \tag{13}$$

[3] The limit of $k_B T \gg k_B T_1$ is not applicable here, since ξ^{-1} is fairly large. However, this limit of the model could be relevant close to a change from a second- to first-order transition at low T, and it gives interesting non-Fermi-liquid behaviour.

where $\eta \approx 2.70$ and the other quantities were defined previously. Over this temperature range, scattering is dominated by the dynamic fluctuations associated with the diffusive relaxation described above.

If the scattering rate of equation (13) is inserted as the current-relaxation rate $\tau_{\rm el}^{-1}$ in the Boltzmann expression for the electric current, then the anomalous T-dependence of $\rho(T)$ observed in MnSi is obtained (vertex corrections are not expected to play a major role, as discussed below). Equation (13) is the main result of the paper.

The coefficient in front of the $T^{3/2}$ term in the resistivity is observed to decrease slowly with pressure above $P_{\rm C}$ (it decreases by a factor of two in going from $P_{\rm C}$ to $2P_{\rm C}$). It is clear that equation (13) is consistent with this result, since the coefficient is proportional to $J^2\xi^3$ and both ξ and J^2 are expected to decrease gradually with pressure above $P_{\rm C}$ (note that equation (13) is independent of q_0). The observed pressure dependence is so weak, however, that variation in D and in the Fermi-surface parameters might also contribute.

In order to establish constraints on the parameters D and q_0, I consider the experimental temperature range over which the $T^{3/2}$-dependence is seen. For pressures between $P_{\rm C}$ and $2P_{\rm C}$, the $T^{3/2}$-behaviour was reported [1] for temperatures ranging from the minimum measurable temperature of 50 mK up to at least 6 K. If the results above are to be consistent with the data then it is required that $T_0 < 50$ mK and $T_1 > 6$ K over the stated pressure range. Using the measured static susceptibility and the fact that $q_c \leqslant k_f$, the condition on T_1 at $2P_{\rm C}$ implies that $D > 7 \times 10^{-5}$ eV Å^2. Also, comparing the condition on T_0 at $P_{\rm C}$ with that on T_1 at $2P_{\rm C}$ and vice versa, one can set a lower limit on the length scale q_0^{-1} given by

$$q_0^{-1}(P_{\rm C}) > k_f^{-1}\sqrt{\frac{\chi^{-1}(P_c)}{\chi^{-1}(2P_{\rm C})}\frac{6\ {\rm K}}{50\ {\rm mK}}} \approx 16k_f^{-1} \tag{14}$$

and similarly, $q_0^{-1}(2P_{\rm C}) > 7k_f^{-1}$ (I have taken D to be independent of pressure). The length scale of the droplet must be considerably larger than a lattice constant if the results given here are to be compatible with the resistivity data. Of course, it was assumed that $q_0^{-1} \gg k_f^{-1}$ in the original derivation of equations (3) and (4). Thus the experimentally determined requirement, equation (14), is consistent with the basic assumption of the present model.

There are a number of approximations made in the development of equation (13) that should be clarified. First, Landau damping was ignored at all temperatures. Since Landau damping is linear in q, it must dominate over the $Dq_{\rm n}^2$ diffusion term at sufficiently small q, which could be expected to result in a restoration of Fermi-liquid behaviour at low T. The case in which both Landau damping and diffusive relaxation are important is difficult to treat without some microscopic understanding of the $Dq_{\rm n}^2$ term. I shall thus attempt only to demonstrate that a Landau damping term, if included as an additive spin relaxation mechanism in equation (4), would not have a significant effect on the resistivity in the $T^{3/2}$ regime. The value of the coefficient determining the magnitude of Landau damping was determined by LT for MnSi to be $\gamma = 2.6 \times 10^{-6}$ eV Å. From the above lower-limit estimate for D, it is found that Landau damping would only be expected to provide the dominant scattering mechanism when $q_{\rm n} \ll \gamma/D \approx 0.03$ Å^{-1}. Since such small momentum transfers, i.e. those for which $q \ll k_f$, have little effect on the electric current, they are not expected to influence the resistivity. In other words, the inclusion of vertex corrections to the current-relaxation rate is expected to remove the contribution of those q for which Landau damping is important. This justifies the omission of Landau damping above while reducing the status of the model spin susceptibility, equation (3), to that of a model applicable only to calculations of *transport* properties, or other properties for which the effects of such small q can be ignored.

As implied in the previous paragraph, the substitution of equation (13) into the Boltzmann expression for the resistivity corresponds to a neglect of vertex corrections to the

current–current correlation function. Vertex corrections are not expected to be crucial [15] when the typical scattering event that contributes to the imaginary part of the self-energy is such that it effects a significant change in the electron velocity $\mathbf{v_p}$. Since the q integral in equation (7) is dominated by $q \approx q_c \leqslant k_f$ in the case for which the $T^{3/2}$ behaviour occurs, vertex corrections are expected to play a relatively minor role. Here it is also interesting to note that bandstructure studies of MnSi have revealed that its Fermi surface offers an unusually large phase space for small-q scattering events in which $\mathbf{v_p}$ changes significantly. (This has been pointed out in [16], see also [17], and is due to the fact that the Fermi surface includes a pair of large open sheets that remain very close together throughout the Brillouin zone so that interband scattering events, which can result in a significant change of $|\mathbf{v_p}|$ and $\hat{\mathbf{v}}_\mathbf{p}$, are likely to occur.) This may give some indication as to what are the properties peculiar to MnSi that give rise to the anomalous transport behaviour described in this paper.

Finally, it should be acknowledged that, without independent estimates of the parameters D and q_0, it is impossible to say whether the predicted crossover temperature T_0 is low enough to account for the observed non-Fermi-liquid behaviour in MnSi. However, the main point of this article is that for suitable values of D and q_0, the *correct* temperature dependence of $\rho(T)$ is obtained. In comparison, the model of LT (i.e. the model in which $\Gamma_\mathbf{q}$ in equation (3) is taken to have the Landau-damping form) also predicts Fermi-liquid behaviour below a crossover temperature T^* with non-Fermi-liquid behaviour occurring above this temperature. The authors of [1] observed that T^* can be estimated from experiment and is found to be more than an order of magnitude too large to explain the data. It should also be emphasized that, even if T^* *had* been sufficiently low, the $\rho(T)$ predicted by the LT model would not be proportional to $T^{3/2}$ over any substantial temperature range [1, 14]. Thus the value of the present work is that a qualitatively correct description of $\rho(T)$ has been obtained starting from a simple physical picture of the paramagnetic phase near P_C.

In summary, I have developed a theoretical model of the electrical resistivity near a weakly first-order phase transition to ferromagnetism. I have shown that the unusual temperature dependence observed in the low-T resistivity of MnSi can be explained by identifying the main source of electron scattering as dynamic fluctuations in the spin density, which are treated using a spin-diffusion model. The phenomenological description presented here may be useful as a first step towards understanding the high-pressure phase in MnSi, especially given the close connection to well-known models of itinerant ferromagnets that should be applicable in the ordered state. However, a better understanding of the spatial structure of the spin system at low T and pressures above P_C is needed.

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