Small-angle interband scattering as the origin of the $T^{3/2}$ resistivity in MnSi

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A possible explanation is given for the anomalous $T^{3/2}$ temperature dependence of the electrical resistivity of MnSi, which is observed in the high-pressure paramagnetic state. The unusual Fermi surface of MnSi includes large open sheets that intersect along the faces of the cubic Brillouin zone. Close to these intersections, long-wavelength interband magnetic spin fluctuations can scatter electrons from one sheet to the other. The current relaxation rate due to such interband scattering events is not reduced by vertex corrections as is that for scattering from intraband ferromagnetic fluctuations. Consequently, current relaxation proceeds in a manner similar to that occurring in nearly antiferromagnetic metals, in which low-temperature $T^{3/2}$ behavior is well known. It is argued that this type of non-Fermi-liquid behavior can, for a metal with ferromagnetic fluctuations near Fermi sheet intersections, persist over a much wider temperature range than it does in nearly antiferromagnetic metals.

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I. INTRODUCTION

Much recent attention has been paid to the itinerant helimagnet MnSi\cite{1,2,3,4,5,6,7,8,9,10,11}. The ordered state occurs at low pressure, and is characterized by a helical spiral with a period of 180 Å, making the system nearly ferromagnetic on atomic length scales. Current interest is mainly in properties of the system observed at high pressure, outside the helimagnetic dome in the $P - T$ phase diagram. For example, at pressures above the critical value $P_C = 14.6$ Kbar required to kill the helimagnetism at $T = 0$, the electrical resistivity has been found to vary with temperature as $\rho(T) = \rho_0 + aT^{3/2}$. This non-Fermi liquid (NFL) behavior, which is the subject of this article, persists down to the lowest measured temperature of below 40 mK and up to the highest applied pressure of greater than 2$P_C$. It is in apparent disagreement with the standard picture of nearly magnetic metals\cite{12,13,14} according to which the predicted low-$T$ NFL resistivity\cite{15,16} varies as $T^{5/3}$ close to a transition to ferromagnetism. Also at pressures well above $P_C$, neutron scattering measurements have revealed a novel type of long-range magnetic order\cite{17}. A recent theoretical proposal\cite{18} describes this so-called partial order as a complex 3D spin configuration within a large (180Å) cubic supercell that is periodically repeated. The variation of the direction of the local magnetization occurs on the length scale of the supercell so spins are aligned over distances significantly larger than the atomic spacing.

The NFL behavior is seen both when the partial order is present and when it is absent. This suggests that the $T^{3/2}$ dependence might be explained using a simple model that contains long-wavelength spin fluctuations, which appear to remain well above $P_C$, without worrying about the actual spin configuration. Since there are no other known ferromagnets (or long wavelength helimagnets) that exhibit $T^{3/2}$-resistivity in the non-magnetic state\cite{19}, peculiarities of the MnSi band structure also deserve attention. Recent theoretical bandstructure work\cite{20} shows that the Fermi surface of MnSi has unusual features related to large intersecting Fermi surface sheets that provide ample phase space for small wavevector interband scattering.

In this article I show that the observed $T^{3/2}$ behavior of the electrical resistivity is expected if long-wavelength magnetic fluctuations that couple spins on the intersecting Fermi surface sheets play a significant role as scatterers. This result follows from the simplest model of a nearly-ferromagnetic system along with consideration of key features in the MnSi Fermi surface. The main assumption is that MnSi has a tendency towards long-wavelength interband magnetic correlations at pressures above $P_C$. I should emphasize that no attempt is made here to explain the magnetic state of MnSi. Rather I simply assume that long wavelength spin correlations persist over a wide range of pressure above $P_C$ and then predict their effect on current relaxation.

I begin by reviewing the MnSi Fermi surface and then give the qualitative explanation for the temperature-dependent resistivity. An explicit calculation of the resistivity, based on a single-particle effective scattering rate, follows below and some discussion of temperature crossovers away from the $T^{3/2}$ regime is given near the end of the article.

Jeong and Pickett\cite{21} (also see Ref. 17) describe the Fermi surface of MnSi as consisting of three sheets: one is a $\Gamma$-centred pocket (that is not discussed here) and the other two are “jungle gym” open sheets with necks on the faces of the cubic Brillouin zone. The latter two, which I label $\alpha$ and $\beta$ as in Fig. 1, intersect one another at the cube faces, thus sharing an elliptical intersection with the boundary plane. (The degeneracy at points on the cube face is protected by the symmetry of the B20 crystal\cite{22}). Interestingly, the normal of each sheet makes an angle with the normal to the cube face that is not equal to $\pi/2$. Translational symmetry is nonetheless preserved since one sheet merges smoothly into the other as the cubic face is crossed. An illustrative cross-section\cite{23} of the $\alpha$ and $\beta$ sheets is shown on the left side of Fig. 1 and a zoom on their intersection is shown in the upper right. At their intersection, the Fermi velocities for the two sheets point in different directions\cite{24}, making an angle $2\eta$ in Fig. 1. Given the intimate connection between the $\alpha$ and $\beta$ sheets, it seems likely that strong interband spin correlations at the $\alpha - \beta$ intersection will exist whenever interband correlations do.

If long-wavelength spin fluctuations that couple spins on the $\alpha$ and $\beta$ sheets are important, then the k-space region shown in the zoom of Fig. 1 is of special interest for trans-
FIG. 1: Colour online. Left: 2D section of Brillouin zone showing the α and β jungle gym sheets of the MnSi Fermi surface as inner and outer curves, respectively (red and blue, respectively, in colour version). The section is indicated by a dashed line on cube in the lower right. Upper right: Zoom view of the intersection of α and β sheets. Arrows on left figure represent velocity while on the right a typical small-q interband scattering process is shown. The thicker lines of the F.S. have higher electron density in the applied field $E \parallel \hat{k}$.

Lower right: Surface of Brillouin zone with elliptical $\alpha - \beta$ intersections indicated on cube faces. Fig. 1 is meant to illustrate qualitative features and is not quantitatively accurate. Compare to Fig. 7 of Ref. 5.

Here, an electron can be scattered by a small-q interband fluctuation from one sheet to the other. Since the Fermi surface velocities make a finite angle at the intersection, the current of the scattered electron changes significantly when this happens. Thus, unlike scattering from intraband small-q spin fluctuations, the effect of interband scattering on current transport does not vanish with $q^2$ due to the $1 - \cos \theta$ vertex factor. For similar reasons, the Landau damping frequency of the spin fluctuations is independent of $q$, rather than linear in $q$ as it is for intraband fluctuations.

It becomes apparent that the phase-space for scattering by interband ferromagnetic spin-fluctuations in MnSi is similar to that for scattering from spin fluctuations in a nearly antiferromagnetic 3D metal. In both cases there is a line of points on the F.S. (the $\alpha - \beta$ intersections play the role of the hot spots) near which electrons are susceptible to scattering by small-$q$ fluctuations in the order parameter. The damping rate of the spin fluctuation is independent of $q$ and the scattering process effectively relaxes the current when $q = 0$. It is therefore not surprising that a $T^{3/2}$ term in the resistivity, which is well-known for nearly antiferromagnetic-metals, $^{12,13,20,21}$ should also occur in MnSi.

The simple preceding argument captures the main qualitative result of this article. I now calculate the $T^{3/2}$ coefficient, taking advantage of the analogy with the antiferromagnetic case. To describe the long wavelength spin fluctuations I adopt the following model spin-susceptibility $^{16}$

$$\chi(q, \omega) = \frac{c}{-i\omega/\omega(q) + \xi^2 + q^2}, \quad (1)$$

The dimensionless correlation length $\xi$ (distances are in units of lattice constants and $\hbar = 1$ unless otherwise stated) is assumed to be much larger than unity and independent of $T$ at low $T$. The Landau damping frequency $\omega(q)$ is discussed below and $c$ is a constant. In this article, the temperature range of interest is that for which the factor $\omega(q)/(q^2 + \xi^2)$ is much smaller than a typical thermal frequency $\omega$ at small $q$ and much larger than it for $q = 1$.

Explicit Fermi sheet labels are now introduced (spin labels are never used in this letter) in the calculation of the Landau damping rate. (The main interest is interband scattering near the $\alpha - \beta$ intersection; expressions are general enough to include the intraband calculation but the latter is done roughly, i.e. for an isotropic band.) From the bubble diagram for the susceptibility with one electron Green’s function having momentum $\mathbf{k}$ on Fermi sheet $\nu$ and the other momentum $\mathbf{k} + \mathbf{q}$ on Fermi sheet $\nu'$, the Landau damping frequency is found to satisfy

$$\omega_{\nu'\nu}(\mathbf{q}) \propto \left[ \int_{\nu'} \frac{dS_{\mathbf{k}}}{v_{\mathbf{k}}} \delta(\mathbf{v}_{\mathbf{k} + \mathbf{q}} \cdot (\mathbf{k} + \mathbf{q}) - \epsilon_f) \right]^{-1}. \quad (2)$$

where the integral is over the vth sheet of the Fermi surface, $v_{\mathbf{k}}$ is the Fermi velocity at $\mathbf{k}$ on the vth sheet and $\epsilon_f$ is the Fermi energy.

For the intraband case $\nu = \nu'$, Eq. 2 gives $\omega_{\nu\nu}(\mathbf{q}) \propto q$ for small $q$, while for interband fluctuations involving non-intersecting Fermi sheets the integral is zero for $q$ smaller than the narrowest separation of the Fermi sheets. But if distinct sheets $\nu$ and $\nu'$ share a line of points $\mathbf{k}$ at which $v_{\mathbf{k}} \neq v_{\nu'\mathbf{k}}$, as the $\alpha$ and $\beta$ sheets do in MnSi, then the Landau damping rate is finite for $q = 0$. For the Fermi surface of Fig. 1, the $q = 0$ value of the integral in Eq. 2 is $6\pi k_f/(v_f^2 \sin 2\eta)$ where $2\pi k_f$ is the circumference of the elliptical $\alpha - \beta$ intersection and $v_f$ is the magnitude of the Fermi velocity at this intersection, taken to be the same for both sheets.

The Landau damping rate is $q$ independent for long wavelength interband spin fluctuations in MnSi. In this regard they resemble antiferromagnetic spin fluctuations for which small deviations away from the ordering wavevector $Q$ do not affect the damping rate.

Having the spin fluctuation propagator from Eq. 1 the quasiparticle scattering rate may be calculated to lowest order from the self energy diagram containing this propagator and a free electron Green’s function. However, the current relaxation rate cannot be set equal to the quasiparticle scattering rate for nearly ferromagnetic systems because vertex corrections to low-$q$ processes are important. Since I am to use a relaxation-time approximation to the Boltzmann equation, some vertex correction factor must be inserted into the momentum integrand of the self-energy in order to account for the fact that certain scattering processes do not alter the current. I use the vertex correction factor appropriate for elastic scattering, which is

$$\Lambda_{\nu'\nu}(\mathbf{q}) = 1 - \frac{v_{\nu'\mathbf{k}} \cdot \hat{u}}{v_{\mathbf{k}} \cdot \hat{u}}. \quad (3)$$
the applied field. Directions for which \( \mathbf{v}_k \cdot \mathbf{u} = 0 \) are of no concern since they do not contribute to the current.

The presence of \( \Lambda_{qf}(\mathbf{q}) \) results in an extra factor of \( q^2 \) in the \( q \) integral for intraband scattering. (The term that is linear in \( q \) in Eq. [3] vanishes in the angular integral over \( \mathbf{q} \).) A similar \( q^2 \) factor occurs for scattering by acoustic phonons.

For interband scattering between the \( \alpha \) and \( \beta \) sheets close to their intersection, the vertex correction \( \Lambda_{qf}(\mathbf{q}) \) is zero for the four cube faces that are parallel to \( \mathbf{u} \) since the velocity component parallel to the field is equal for the two sheets on these faces. On faces perpendicular to \( \mathbf{u} \) interband scattering reverses the velocity along the field, as seen in Fig. 1, so \( \Lambda_{qf}(0) = 2 \).

Since \( \Lambda_{qf}(0) \) is large, interband scattering on the faces orthogonal to \( \mathbf{u} \) relaxes the current even when \( q = 0 \). Again this is similar to antiferromagnetic fluctuations, which effect a large velocity change by scattering an electron through \( \mathbf{Q} \).

It seems unlikely that a better treatment of vertex corrections would change this qualitative result. A contribution to the current by electrons on cube faces perpendicular to \( \mathbf{u} \) is possible in MnSi because the \( \alpha \) and \( \beta \)-sheet normals do not lie in the plane of the zone boundary. Generic open Fermi surfaces have normals parallel to the faces at the boundary, which makes scattering on faces perpendicular to the field irrelevant to transport in most metals.

The momentum integral in the interband self-energy calculation may be carried out using coordinates shown in the zoom of Fig. 1. A convergent Fermi surface integral of a function of \( q \) is done as \( \int dS_{qf}(q) = 2\pi \int q dq |q| \left( \sqrt{q^2 + k^2 \sin^2 \eta} \right) \).

I define \( \xi_{\nu\nu}(k) = \xi_{\nu\nu}^2(0) + k^2 \sin^2 \eta \) where the interband correlation length \( \xi_{\nu\nu}(0) \) is expected to be different from the corresponding intraband quantity \( \xi_{\nu\nu}(k) = \xi_{\nu\nu}(0) \), but to share the general features noted above. Also, \( \xi_{\nu\nu}(k) \) is much larger than \( k_B T / \omega_{\nu\nu}(0) \) when \( k \) is of order unity.

The current relaxation rate \( \tau_{\nu\nu}^{-1}(k, \omega) \) associated with the scattering of electrons from band \( \nu \) with momentum \( \mathbf{k} \) and energy \( \omega \) to any momentum or energy on band \( \nu' \) is given at zero temperature by

\[
\tau_{\nu\nu}^{-1}(k, \omega) = g_{\nu\nu} \int_0^\omega \frac{d\omega'}{\omega'} \frac{\Lambda_{qf}(q) \omega_{\nu\nu}(q)}{v_f e^2 + \omega_{\nu\nu}(q) \xi_{\nu\nu}^2(k) + q^2}.
\]

(4)

where \( g_{\nu\nu} \) is a constant energy coupling. The angular integral has removed directional dependence so that, for example, \( \Lambda_{qf}(q) = 1 - \mathbf{v}_k \cdot \mathbf{v}_k = q^2 / 2 \).

The frequency dependence of Eq. [4] can be found by power counting. The intraband case has \( \Lambda_{qf}(q) \propto q^2 \) and \( \omega_{\nu\nu}(q) \propto q \) while \( \xi_{\nu\nu}^2(k) \) is a constant much smaller than unity. The second term in the denominator of the \( q \) integral goes as \( q^6 \) so powers of \( \omega \) are assigned according to \( q \propto \omega^{1/3} \). Thus the \( q \) integral goes as \( \omega^{-1/3} \) and \( \tau_{\nu\nu}^{-1}(k, \omega) \propto \omega^{2/3} \). This is a well known result for current relaxation near a ferromagnetic transition.

In the case of interband scattering both \( \Lambda_{qf}(q) \) and \( \omega_{\nu\nu}(q) \) are constant for small \( q \) and the \( q \) integral depends on \( k \) through \( \xi_{\nu\nu}(k) \). At the \( \alpha - \beta \) intersection, the current relaxation rate is

\[
\tau_{qf}^{-1}(0, \omega) = \frac{\pi g_{qf} \omega}{2 v_f}.
\]

(5)

while far from the \( \alpha - \beta \) intersection it is approximately given by

\[
\tau_{qf}^{-1}(k, \omega) = \frac{g_{qf} \omega^2}{v_f k_B T_0} \quad k \approx k_f
\]

(6)

where \( k_B T_0 \approx k_f^2 \omega_{qf}(0) \) (recall that the temperature range of interest lies well below \( T_0 \)). The situation is identical to that of nearly antiferromagnetic metals: the relaxation rate is linear in \( \omega \) at hot spots and quadratic in \( \omega \) elsewhere. More precisely, the relaxation rate is linear in \( \omega \) when \( \omega_{qf}(k) \xi_{\nu\nu}^2(k) \ll \omega \). The basic assumption of this work is that, for MnSi, there exists a low-temperature regime at pressures well above \( P_C \) where this condition is satisfied by thermal \( \omega \) and \( k \) sufficiently close to the \( \alpha - \beta \) intersection.

A relaxation-time approximation is used to calculate \( \rho(T) \). This is valid at low \( T \), where the impurity scattering rate \( \tau_{el}^{-1} \) exceeds the inelastic scattering rate, in nearly antiferromagnetic metals. Since the calculation of the resistivity proceeds exactly as in the antiferromagnetic case (described in the Appendix of Ref. [22] for example), I only sketch it briefly.

The nonequilibrium part of the quasiparticle distribution \( \delta n_{\nu k} \) in an applied field \( \mathbf{E} = e\mathbf{E} \) is assumed to be

\[
\delta n_{\nu k} = e\mathbf{E} \delta n_{\nu k} \mathbf{v}_{\nu k} \cdot \mathbf{u} \frac{1}{\tau_{in}^{-1}(k, \epsilon_f) + \tau_{el}^{-1}}.
\]

(7)

with the resulting current

\[
\mathbf{j} = e \sum_{\nu k} \delta n_{\nu k} \mathbf{v}_{\nu k}.
\]

(8)

Band-labels have been dropped from the inelastic scattering rate \( \tau_{in}^{-1}(k, \epsilon_f) \) since interband scattering is assumed and the energy argument identifies the initial band. The Fermi function is written as \( n_0 \).

To lowest order in \( \tau_{in}^{-1}(k, \epsilon_f) \tau_{el}^{-1} \), Eq. [8] gives

\[
\frac{\rho(T) - \rho(0)}{\rho(0)} = \rho(0) \sigma_1(T)
\]

(9)

where

\[
\sigma_1(T) = \frac{2 e^2 \tau_{el}^{-2}}{(2\pi)^3} \sum \int d\omega \left( -\frac{dn_0}{d\omega} \right) \int d\mathbf{k} \frac{dS_k}{v_{\nu k} \tau_{in}^{-1}(k, \epsilon_f)}.
\]

(10)

I substitute Eq. [4] into Eq. [10] and note that the \( k \) integral converges within a strip of width \( k_f \sqrt{T/T_0} << k_f \) about the \( \alpha - \beta \) intersection. The result, written in standard units, is

\[
\sigma_1(T) = \frac{\Gamma n e^2 \tau_{el}^{-1} (T / T_0)^{3/2}}{m (T / T_0)^{3/2}}
\]

(11)

where

\[
\Gamma = \tan \eta \frac{g_{qf}}{\hbar \tau_{el}^{-1}} \left( \frac{k_B T_0}{\epsilon_f} \right)
\]

(12)

to within a factor of order unity and \( n/m = \epsilon_f k_f / (\hbar \pi)^2 \), \( \epsilon_f = \hbar v_f k_f \). Similar to the antiferromagnetic case, there
is a crossover to Fermi liquid behaviour for $T < T_c$ where $T_c = k^2 T^2 f^{-1} T^0 0 << T_0$. This means that $(T_0/T_c) = k^2 T^2 f^{-1} T^0 0$ is the largest temperature range over which $T^{3/2}$-resistivity can occur in this model. The data, which show $T^{3/2}$ resistivity spanning two decades at $P = 2P_C$, thus require that the interband spin correlation length at the $\alpha - \beta$ intersection is at least of order ten atomic spacings at this pressure. Although it would be unusual, the existence of such long spin correlations well away from critical pressure is not implausible in MnSi, especially given that Binz et al’s model of the partially ordered state above $P_C$ appears to have static ferromagnetic spin correlation lengths of the required order.

The $k$-averaged inelastic relaxation rate in Eq. (10) emerges from the expansion in small $\tau^{-1}_{\alpha \beta}(k, \epsilon_f)$. However, if one uses the crude procedure of simply replacing $\tau^{-1}_{\alpha \beta}(k, \epsilon_f)$ by its $k$-average in the vicinity of the $\alpha - \beta$ intersection, then the calculation may be done as above without assuming that impurity scattering is dominant. The result is $\rho(T) \propto T^{3/2}$ even when $\tau^{-1}_{\alpha \beta}(0, k_g T) >> \tau^{-1}_{\alpha \beta}(0)$. The general statement is that $T^{3/2}$-resistivity occurs when current relaxation is dominated by scattering from long-wavelength interband spin fluctuations near the $\alpha - \beta$ intersection.

For nearly antiferromagnetic metals, one expects $\rho(T) - \rho(0)$ to vary as $T^{3/2}$ only for temperatures low enough that $\rho(T) - \rho(0) << \rho(0)$ (this agrees with recent data on heavy fermion metals[22-23]). This is because the $T^{3/2}$-dependence only occurs while the impurity scattering rate is sufficient to replenish the nonequilibrium density at hot spots. At higher $T$, the nonequilibrium density is removed from hot spots by rapid inelastic scattering and the resistivity is determined by scattering that occurs elsewhere on the Fermi surface. On the other hand, measurements of MnSi see $T^{3/2}$ behavior up to temperatures for which $\rho(T) >> \rho(0)$. This raises the question of how could scattering at $\alpha - \beta$ intersections remain important if impurity scattering is unable to maintain the nonequilibrium density at these intersections.

A proper answer to this question would likely require a Boltzmann-equation analysis as done in Ref. 22 for antiferromagnetic metals, but an obvious suggestion is the following: scattering by intraband fluctuations replenishes the electron distribution near the $\alpha - \beta$ intersection while having little effect on the current. I elaborate on this before concluding. Interband scattering tends to equilibrate the densities on the $\alpha$ and $\beta$ sheets at their intersection. Intraband scattering counters this effect by redistributing electrons along each sheet in an effort to equilibrate the density at the intersection with that far from it. This intraband redistribution process can be effective even when current relaxation by intraband scattering is not. (Consider that interband scattering tends to cause the electron density at the intersection to vary on the scale $\delta k \approx k_f(T/\rho)^{1/2} << k_f$ along the Fermi surface throughout the $T^{3/2}$ regime. Intraband scattering processes with momentum transfer $q \ll k_f$ could prevent this tendency, at least up to temperatures approaching $T_0$, while having negligible effect on the current.) It thus seems possible that intraband scattering could be responsible for the robustness of the $T^{3/2}$ behavior in MnSi. I leave a detailed study of the interplay between intraband and interband scattering near Fermi sheet intersections to future work.

In summary, I have presented a potential explanation for non-Fermi liquid resistivity in MnSi that is based on the usual model of a nearly ferromagnetic metal but takes into account unusual features of the Fermi surface. The work suggests that interband spin correlations near the Fermi sheet intersections are important in MnSi, and that their effect on other properties should be considered. I thank A. Boonchun and P. Pairor for useful discussions.

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