Residual resistivity of FeGe under pressure

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Residual resistivity of FeGe under pressure exhibits an anomaly at a critical pressure $p_c \approx 19$ GPa whose origin is not understood. In previous theoretical work, it has been suggested that at the critical pressure a minority spin band starts to become occupied in FeGe. Here we provide further support for this scenario by studying, within the standard Boltzmann-type transport theory combined with a T-matrix treatment of scattering on dilute point defects, how the residual resistivity of a helical ferromagnet changes with exchange splitting.

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I. INTRODUCTION

Much attention has been paid recently to two seemingly unrelated isostructural and isoelectronic compounds, namely the magnetically ordered metal FeGe and the anomalous insulator FeSi. FeGe becomes magnetically ordered below 279 K with a large magnetic moment $\sim 1\mu_B$ per Fe atom.[1,2] Due to the lack of inversion symmetry, the weak Dzyaloshinskii-Moriya interaction leads to a formation of long-range spirals[3] with a period of[4] $\sim$700 Å, leading to a rich phenomenology in applied magnetic fields.[5] On the other hand, FeSi is a small-gap insulator with mysterious magnetic properties at high temperatures.[6,7] Interest in this compound has been revived after it has been proposed that FeSi is an example of a Kondo insulator.[8,9] It has also been argued that the gap formation in FeSi represents a simple model for the electronic structure of quasicrystals.[10]

A new perspective on the physics of FeSi has been offered by a seminal study of the $FeSi_{1-x}Ge_x$ alloys[11] which has found a weak first-order transition between a magnetic metal and a paramagnetic insulator at a critical doping x_c. This finding has lent strong support to the point of view that the anomalous magnetic properties of FeSi are caused by its proximity to a nearby ferromagnetic phase.[12] For the sake of completeness, it is worth pointing out that this picture is conceptually similar to the earlier theories proposing the existence of strong ferromagnetic fluctuations in FeSi.[13,14]

The nontrivial point to note here is that since the Ge atoms are larger than the Si atoms, we have to expect that the ratio of the kinetic energy to the Coulomb repulsion energy is smaller in FeGe than in FeSi. Therefore, according to conventional theories, it is FeGe which should be insulating and it is FeSi which should be metallic, exactly opposite to the experimental findings. This anomaly has been explained in Ref. 15 by noting that as regards the magnetic properties, fairly conventional physics is being observed: the more correlated FeGe is magnetically ordered, whereas the less correlated FeSi has a nonmagnetic ground state. This leads then to the natural assumption that it is the magnetism which drives the metal-insulator transition in $FeSi_{1-x}Ge_x$. Since in ordinary cases it is just the other way round, namely the metal-insulator transition is the master and magnetism is the slave, it is very likely that the electronic transition in $FeSi_{1-x}Ge_x$ represents a novel universality class of a metal-insulator transition, which has been dubbed a *magnetically induced metal-insulator transition*.[15]

In an interesting recent study by Pedrazzini *et al.*,[16] the authors have decided to check the highly nontrivial results of Ref. 11 making use of stoichiometric samples. To this end, instead of applying chemical pressure by replacing the Ge atoms in FeGe by the isoelectronic but smaller Si atoms, Pedrazzini *et al*. performed high-pressure measurements with the aim to observe the transition of FeGe at a critical pressure towards an insulating state. Although pressures as large as 30 GPa have been applied, no transition to an insulating state has been observed. However, at a critical pressure $p_c \approx 19$ GPa, anomalies of the resistivity in the limit of low temperatures have been observed. It is the purpose of the present paper to offer a possible explanation of these anomalies.

Our approach is motivated by the results of recent studies of a minimal model for the magnetically induced metal-insulator transition in $FeSi_{1-x}Ge_x$ at zero temperature.[17,18] In those works the weak Dzyaloshinskii-Moriya interaction was neglected and FeGe was modeled as a ferromagnet. It was found that, according to the minimal model, in between the fully polarized metallic magnet and the paramagnetic insulator, there exists a partially polarized metallic phase. In the present work we build on this finding and we will assume that at the critical pressure $p_c \approx 19$ GPa a fully polarized magnet becomes partially polarized. Our goal is to check whether this phenomenology can explain the observed transport anomalies. We would like to emphasize that although motivated by Refs. 17 and 18, our results are, to a large extent, independent of them. In particular, our phenomenology might apply also to the quite different microscopic model of Ref. 19, since simulations of its 1D version also found partially polarized states close to the metal-insulator transition.[20] Moreover, also recent *ab initio* calculations have found a decreasing magnetic moment for pressures close to p_c.[21,22] Our picture seems to be consistent also with the *ab initio* studies of metamagnetism in FeSi which find, in between the paramagnetic insulator and the large-moment metal, a small-moment metallic phase at intermediate magnetic fields.[23]

In Ref. 16 the low-temperature resistivity ρ has been fitted according to $\rho(T) = \rho_0 + AT^n$, where T is the temperature. The residual resistivity ρ_0, as well as the coefficient A and exponent n characterizing the inelastic scattering, have been studied as functions of applied pressure. The following have been found:

(i) The residual resistivity ρ_0 is roughly constant at pressures $p < p_c$. In the vicinity of p_c, there is a resonant-like anomaly of ρ_0. Finally, for $p > p_c$ the residual resistivity ρ_0 increases with applied pressure.

(ii) The inelastic part of the resistivity has a canonical Fermi-liquid form AT^2 at pressures $p < p_c$, and the coefficient A grows only very weakly with the applied pressure in this range. For pressures in the vicinity of p_c and above, the absolute value of the inelastic part increases dramatically and the exponent changes from $n = 2$ to $n \approx 1.5$.

In this paper we concentrate on the observation (i). For the sake of completeness, at this point we just mention that the observation (ii) seems to be perfectly consistent with our picture. In fact, if we imagine describing FeGe by a Hubbard-like model with an on-site interaction U, then a fully polarized state is effectively noninteracting and its resistivity should not exhibit any contribution from electron-electron scattering. Of course, the presence of small but nonvanishing nonlocal interactions does lead to a finite (but small) electron-electron scattering even in this case. The situation changes dramatically at $p > p_c$, where up-spin electrons do scatter on the down-spin electrons and vice versa, even if only the on-site interaction U is retained. This explains the increase of the absolute value of the inelastic resistivity in a very natural way. As regards the change of the exponent n, the situation is more involved and requires a careful examination which will be presented elsewhere. At this point let us only mention that it might be important to take into account that the transition from fully to partially polarized states is a $T = 0$ quantum critical transition associated with a soft longitudinal spin-wave mode.[24] It is worth pointing out that a somewhat similar picture based on spin-disorder scattering has been suggested in Ref. 22.

The plan of this paper is as follows. In Sec. II we show that, due to the long-range spiral structure, even pure potential scattering is off-diagonal in the spin index. In Sec. III we derive, within the Boltzmann transport theory, a formula for the resistivity of an arbitrarily polarized state with off-diagonal scattering on a dilute set of point defects. In Sec. IV we calculate, by a matrix generalization of the Lippmann-Schwinger equation, exact T matrices for such scattering, which we then use in the formula for the resistivity. Finally in Sec. V we present our conclusions.

II. OFF-DIAGONAL SCATTERING

In this section we show that due to the long-range spiral structure, even pure potential scattering is off-diagonal in the spin index. In order to proceed, let us assume that the magnetic field spirals along the spatial z direction according to $\mathbf{B} = B(\cos qz, \sin qz, 0)$. We aim at the simplest possible description and therefore we assume that the Hamiltonian describing the electron spinors is

$$H = -\frac{\hbar^2}{2m}\Delta + \frac{J}{2}\begin{pmatrix} 0 & e^{-iqz} \\ e^{iqz} & 0 \end{pmatrix},$$

where J is the exchange splitting, which has to be large enough to lead to a fully polarized state in FeGe at ambient pressure. With increasing pressure, we will assume that J decreases. We emphasize that our approach is purely phenomenological. For more microscopic approaches, the reader is referred to, e.g., Refs. 21 and 22.

If we introduce the energy difference $\Delta_{\mathbf{k}} = \varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}$, where $\mathbf{q} = (0,0,q)$, the energy eigenvalues of the electrons are

$$\varepsilon_{\mathbf{k}\lambda} = \frac{1}{2}(\varepsilon_{\mathbf{k}+\mathbf{q}} + \varepsilon_{\mathbf{k}}) + \frac{\lambda}{2}\sqrt{J^2 + \Delta_{\mathbf{k}}^2},$$

where $\lambda = \pm 1$ is the spin index. The corresponding eigenvectors normalized in a volume $\mathcal{V}$ are

$$\psi_{\mathbf{k},\lambda} = \frac{1}{\sqrt{2\mathcal{V}}}\begin{pmatrix} \sqrt{1-\lambda\alpha_{\mathbf{k}}} \\ \lambda e^{iqz}\sqrt{1+\lambda\alpha_{\mathbf{k}}} \end{pmatrix} e^{i\mathbf{k}\cdot\mathbf{r}},$$

where we have introduced the notation

$$\alpha_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{\sqrt{J^2 + \Delta_{\mathbf{k}}^2}}.$$

Having described the states of a perfect crystal, let us proceed with the calculation of their scattering on a point defect described by the Hamiltonian

$$H' = V\delta(\mathbf{x} - \mathbf{R}).$$

A simple calculation shows that the matrix element for scattering on such a potential is

$$|\langle\psi_{\mathbf{k}'\lambda'}|H'|\psi_{\mathbf{k}\lambda}\rangle|^2 = \frac{V^2}{2\mathcal{V}^2}\left[1 + \frac{\lambda\lambda'(J^2 + \Delta_{\mathbf{k}}\Delta_{\mathbf{k}'})}{\sqrt{(J^2 + \Delta_{\mathbf{k}}^2)(J^2 + \Delta_{\mathbf{k}'}^2)}}\right].$$

Note that since the energy scale $\Delta_{\mathbf{k}}$ depends on the electron wave vector $\mathbf{k}$, the matrix element is nonvanishing not only in the spin-conserving channel $\lambda' = \lambda$, but also in the spin-flip channel $\lambda' = -\lambda$.

At this point we take into account that due to the long wavelength of the spiraling,[4] q is small and we can safely assume that $J \gg \Delta_{\mathbf{k}}$. In this limit the electron energy eigenvalues simplify to the standard spin-splitting result $\varepsilon_{\mathbf{k}\pm} \approx \varepsilon_{\mathbf{k}} \pm \frac{J}{2}$.

In the spin-conserving channel the scattering matrix element can therefore be simplified to

$$|\langle\psi_{\mathbf{k}'\lambda}|H'|\psi_{\mathbf{k}\lambda}\rangle| \approx \frac{|V|}{\mathcal{V}},$$

as should have been expected. The central result of this section is that, in the spin-flip channel, the scattering matrix element reads as

$$|\langle\psi_{\mathbf{k}'-\lambda}|H'|\psi_{\mathbf{k}\lambda}\rangle| \approx \frac{|V|}{\mathcal{V}} \times \frac{|\Delta_{\mathbf{k}} - \Delta_{\mathbf{k}'}|}{2J}.$$

Let us estimate now the magnitude of the spin-flip matrix element at the critical point between fully and partially polarized states. If we denote the Fermi wave-vector of the fully polarized state as k_N, then the exchange splitting at the critical pressure p_c can be estimated as $J \approx \frac{\hbar^2 k_N^2}{2m}$. Because of the observed large magnetic moment per Fe atom, we have to take k_N to be comparable to $\frac{\pi}{a}$, where $a \approx 4.7$ Å is the lattice constant of FeGe. If we assume that the vectors $\mathbf{k}$ and $\mathbf{k}'$ lie at the majority-spin and minority-spin Fermi surfaces, respectively, i.e., if $k = k_N$ and $k' = 0$, then we can set $\Delta_{\mathbf{k}} \sim \frac{\hbar^2 k_N q}{m} \gg \Delta_{\mathbf{k}'}$. Making use of these estimates we find that the spin-flip matrix element, compared to the spin-conserving matrix element, is reduced by a factor $\frac{q}{k_N} \sim 10^{-2}$.

From now on, the spiral structure becomes irrelevant and will be completely ignored. Its only effect in the treatment which follows is to replace the simple potential scattering by a matrix in spin space, $H' = \hat{V}\delta(\mathbf{x} - \mathbf{R})$, where

$$\hat{V} = \begin{pmatrix} V & W \\ W^* & V \end{pmatrix}. \tag{1}$$

For the sake of simplicity we will assume that in FeGe there is only one type of typical point defects, such as vacancies or interstitials, with concentration n_{imp}. In other words, we will concentrate only on the most important type of point defects. From the above considerations it follows that $|W|/|V| \sim 10^{-2}$.

III. THE BOLTZMANN EQUATION

In this section we shall derive a formula for the resistivity of a partially polarized metal, while working within the standard transport theory as described in Ziman's textbook.[25] The central object of the theory is the electron distribution function $f_{\mathbf{k}\lambda}$, which in the presence of a small applied electric field E is being sought in the form $f_{\mathbf{k}\lambda} = f^0_{\mathbf{k}\lambda} + \Phi_{\mathbf{k}\lambda}\delta(\varepsilon_{\mathbf{k}\lambda})$.

The unknown function $\Phi_{\mathbf{k}\lambda}$ describing the deviation from the equilibrium distribution function $f^0_{\mathbf{k}\lambda}$ has to satisfy the linearized Boltzmann equation for electrons scattering on point defects

$$-eEv^z_{\mathbf{k}\lambda}\delta(\varepsilon_{\mathbf{k}\lambda}) = \frac{1}{\mathcal{V}}\sum_{\mathbf{k}'\lambda'} W^{\lambda\lambda'}_{\mathbf{k}\mathbf{k}'}[\Phi_{\mathbf{k}\lambda}\delta(\varepsilon_{\mathbf{k}\lambda}) - \Phi_{\mathbf{k}'\lambda'}\delta(\varepsilon_{\mathbf{k}'\lambda'})].$$

Here we have assumed, without loss of generality, that the electric field is applied along the z axis and $v^z_{\mathbf{k}\lambda}$ is the corresponding component of the electron group velocity in the state $\mathbf{k}\lambda$.

The scattering from $\mathbf{k}\lambda$ to $\mathbf{k}'\lambda'$ is elastic; therefore $W^{\lambda\lambda'}_{\mathbf{k}\mathbf{k}'} = P^{\lambda\lambda'}_{\mathbf{k}\mathbf{k}'}\delta(\varepsilon_{\mathbf{k}\lambda} - \varepsilon_{\mathbf{k}'\lambda'})$ and in the Born approximation we have

$$\frac{1}{\mathcal{V}}P^{\lambda\lambda'}_{\mathbf{k}\mathbf{k}'} = \frac{2\pi N_{\mathrm{imp}}}{\hbar}|\langle\psi_{\mathbf{k}'\lambda'}|H'|\psi_{\mathbf{k}\lambda}\rangle|^2,$$

where $N_{\mathrm{imp}} = \mathcal{V}n_{\mathrm{imp}}$ is the total number of point defects in the sample. For our simple model of point defects, this implies $P^{\lambda\lambda'}_{\mathbf{k}\mathbf{k}'} = P^{\lambda\lambda'}$. In particular, in the spin-conserving channel and in the spin-flip channel this reads

$$P^{\parallel} = \frac{2\pi n_{\mathrm{imp}}}{\hbar}V^2, \quad P^{\perp} = \frac{2\pi n_{\mathrm{imp}}}{\hbar}|W|^2.$$

Applying standard procedures, for the conductivity we find[25]

$$\sigma = \frac{2e^2\left(\sum_\lambda \oint_\lambda \frac{d^2k}{v_{\mathbf{k}\lambda}} v^z_{\mathbf{k}\lambda}\Phi_{\mathbf{k}\lambda}\right)^2}{\sum_{\lambda\lambda'}\oint_\lambda \frac{d^2k}{v_{\mathbf{k}\lambda}}\oint'_\lambda \frac{d^2k'}{v_{\mathbf{k}'\lambda'}} P^{\lambda\lambda'}_{\mathbf{k}\mathbf{k}'}(\Phi_{\mathbf{k}\lambda} - \Phi_{\mathbf{k}'\lambda'})^2},$$

where the symbol $\oint_\lambda d^2k$ denotes a surface integral along the Fermi surface for spin component λ.

So far, our treatment of the linearized Boltzmann equation has been exact. As shown in Ref. 25, the expression for σ is maximized by the true solution $\Phi_{\mathbf{k}\lambda}$ of the Boltzmann equation. Therefore we will estimate the conductivity from the customary variational solution $\Phi_{\mathbf{k}\lambda} = eE\tau_\lambda v^z_{\mathbf{k}\lambda}$ with the relaxation times τ_λ for the two spin projections taken as variational parameters to be optimized.

If we introduce densities of states at the chemical potential μ for the two spin projections

$$N^0_\lambda(\mu) = \frac{1}{(2\pi)^3\hbar}\oint_\lambda \frac{d^2k}{v_{\mathbf{k}\lambda}},$$

then the optimal relaxation times τ_λ which maximize σ are easily found to be given by the expressions

$$\tau_\lambda = \frac{1}{P^{\parallel}N^0_\lambda(\mu) + P^{\perp}N^0_{-\lambda}(\mu)}. \tag{2}$$

Note that the scattering rates τ^{-1}_λ have a simple interpretation, being sums of intraband and interband scattering probabilities.

Let us further assume that the Fermi surfaces are spherical. In that case we have $N^0_\lambda(\mu) = \frac{m_\lambda k_\lambda}{2\pi^2\hbar^2}$, where k_λ and m_λ are the Fermi wave vector and the effective mass for spin λ, respectively. Plugging Eq. (2) into the formula for σ, the total conductivity can be written in a natural form as a sum of the Drude conductivities for the individual spin projections:

$$\sigma = \frac{n_\uparrow e^2\tau_\uparrow}{m_\uparrow} + \frac{n_\downarrow e^2\tau_\downarrow}{m_\downarrow}. \tag{3}$$

In the rest of this paper we will apply Eqs. (2) and (3) to the experimental data. In the partially polarized states the numbers of up-spin and down-spin electrons have to satisfy the condition $n_\uparrow + n_\downarrow = n$. Our goal will be to determine the change of the residual resistivity $\rho_0 = \frac{1}{\sigma}$ between the fully polarized state with $n_\downarrow = 0$ and the partially polarized states with $n_\downarrow > 0$.

IV. *T*-MATRIX DESCRIPTION

In order to go beyond the Born approximation used in the previous section, in the present section we shall study a lattice version[26] of the continuum model discussed in Sec. II and we shall construct an exact solution for scattering off a single point defect described by Eq. (1). We shall assume that the local Green's function of an ideal lattice is diagonal in spin space,

$$\hat{G}_0(\varepsilon) = \begin{pmatrix} G_{0\uparrow}(\varepsilon) & 0 \\ 0 & G_{0\downarrow}(\varepsilon) \end{pmatrix}.$$

The exact T-matrix for scattering off the point defect is then given by the solution of the Lippmann-Schwinger equation[27] generalized to the matrix form

$$\hat{T}(\varepsilon) = \hat{V} + \hat{V}\hat{G}_0(\varepsilon)\hat{T}(\varepsilon).$$

This matrix equation is formally similar to that studied in the theory of dirty superconductors[28] and its solution reads as

$$\hat{T}(\varepsilon) = [\mathbf{1} - \hat{V}\hat{G}_0(\varepsilon)]^{-1}\hat{V},$$

where $\mathbf{1}$ is a 2×2 unit matrix. Performing an explicit matrix inversion, we find

$$\hat{T}(\varepsilon) = \frac{1}{\mathcal{D}(\varepsilon)}\begin{pmatrix} V_\downarrow(\varepsilon) & W \\ W^* & V_\uparrow(\varepsilon) \end{pmatrix},$$

where

$$V_\lambda(\varepsilon) = V - (V^2 - |W|^2)G_{0\lambda}(\varepsilon),$$
$$\mathcal{D}(\varepsilon) = 1 - VG_{0\uparrow}(\varepsilon) - V_\uparrow(\varepsilon)G_{0\downarrow}(\varepsilon).$$

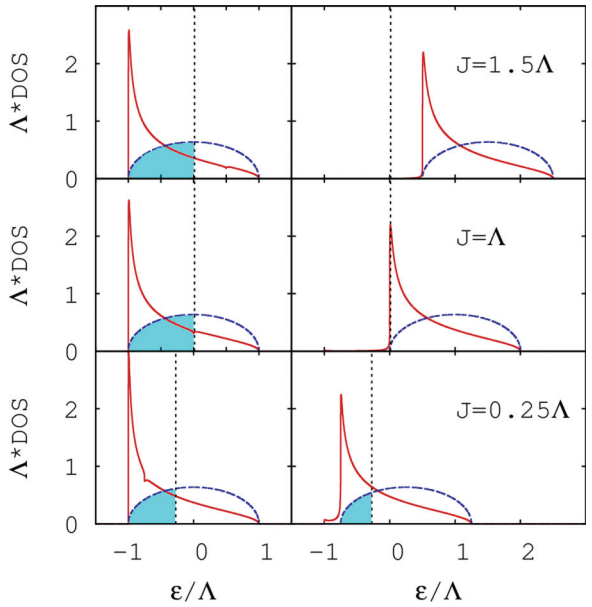

FIG. 1. (Color online) Evolution of the unperturbed density of states $N^0_\lambda(\varepsilon)$ (dashed lines) and of the band occupation (shaded) with changing exchange splitting J. The chemical potential μ is indicated by the vertical dotted line. Left column: Majority band $\lambda = \uparrow$. Right column: Minority band $\lambda = \downarrow$. Also shown is the local density of states at the point defect $A_\lambda(\varepsilon)$ for $V/\Lambda = -0.43$ and $W/V = 0.2$ (full lines).

Note that in the weak-scattering limit $V, W \to 0$ we have $\hat{T} \to \hat{V}$; i.e., the T matrix reduces to the Born approximation. However, for finite $\hat{V}$ the T matrix may develop additional nonperturbative features which are the subject of this section.

In order to proceed we need to specify the form of the unperturbed local Green's function $\hat{G}_0(\varepsilon)$. For the sake of simplicity, let us assume that the density of states for both spin projections is semicircular,

$$N^0_\uparrow(\varepsilon) = \frac{2}{\pi\Lambda^2}\sqrt{\Lambda^2 - \varepsilon^2}, \quad N^0_\downarrow(\varepsilon) = \frac{2}{\pi\Lambda^2}\sqrt{\Lambda^2 - (\varepsilon - J)^2}.$$

Note that we have assumed that the bandwidths of both the majority spins $\uparrow$ and the minority spins $\downarrow$ are the same and equal to 2Λ. The minority band is rigidly shifted upwards by the exchange splitting J with respect to the majority band; see Fig. 1.

In the low-temperature limit which we are interested in, the chemical potential μ has to be determined from

$$\sum_{\lambda=1,2} \int^{\mu} d\varepsilon N^0_\lambda(\varepsilon) = n.$$

For concreteness, from now on we will assume that the band is quarter filled, i.e., that $n = \frac{1}{2}$. In the fully polarized phase (which is realized at large exchange splittings J) the majority band is therefore half filled and the chemical potential is $\mu = 0$ in this case. The quantum phase transition from the fully polarized to the partially polarized state occurs when the bottom of the minority band drops below μ. This happens at the critical value $J_c = \Lambda$; see Fig. 1.

Our choice of $N^0_\lambda(\varepsilon)$ implies that the unperturbed local Green's functions are given by

$$G_{0\lambda}(\varepsilon) = M_\lambda(\varepsilon) - i\pi N^0_\lambda(\varepsilon),$$

where the real part

$$M_\uparrow(\varepsilon) = \mathrm{Re}\left[\frac{2\epsilon}{\Lambda^2}\left(1 - \sqrt{1 - \frac{\Lambda^2}{\varepsilon^2}}\right)\right]$$

is a Kramers-Kronig image of $N^0_\uparrow(\varepsilon)$ and the function $M_\downarrow(\varepsilon)$ is given by the same expression, except for the rigid shift $\varepsilon \to \varepsilon - J$.

A. Local density of states

Before discussing the results for $\hat{T}(\varepsilon)$, let us point out that the local Green's function at the point defect, $\hat{G}(\varepsilon)$, is given by the exact equation[27]

$$\hat{G}(\varepsilon) = \hat{G}_0(\varepsilon) + \hat{G}_0(\varepsilon)\hat{T}(\varepsilon)\hat{G}_0(\varepsilon).$$

This means that the singularities of $\hat{T}(\varepsilon)$ should be reflected also in the Green's function at the point defect.

Since the Green's function $\hat{G}(\varepsilon)$ has a simple physical meaning, it will be studied first. From the exact formula for $\hat{G}(\varepsilon)$ it follows that the spin-resolved spectral functions at the point defect are given by

$$A_\lambda(\varepsilon) = -\frac{1}{\pi}\mathrm{Im}\frac{G_{0\lambda}(\varepsilon)[1 - VG_{0-\lambda}(\varepsilon)]}{\mathcal{D}(\varepsilon)}. \tag{4}$$

Note that for $W = 0$, the majority and minority spin bands decouple and Eq. (4) reduces to

$$A_\lambda(\varepsilon) = \frac{N^0_\lambda(\varepsilon)}{[1 - VM_\lambda(\varepsilon)]^2 + [\pi V N^0_\lambda(\varepsilon)]^2},$$

which is a well-known result for the case of simple potential scattering off an isolated point defect.[27] For sufficiently strong defect potentials V the local density of states $A_\lambda(\varepsilon)$ is known to exhibit large deviations from $N^0_\lambda(\varepsilon)$.

This behavior is preserved also in the case of coupled bands described by Eq. (4), as shown explicitly in Fig. 1 for an attractive defect potential $V/\Lambda = -0.43$, a largish interband coupling $W/V = 0.2$, and several values of exchange splitting J. As is evident from Fig. 1, for $J \approx J_c$ the singularities of $A_\downarrow(\varepsilon)$ are located at $\varepsilon \approx 0$; therefore they are potentially relevant for transport.

In Fig. 2 we plot how the local density of states of the minority band at the defect site $A_\downarrow(\varepsilon)$ depends on the parameters V, W characterizing the defect scattering. The largish value of $W/V = 0.2$ has again been chosen to amplify the effects of interband scattering. It can be seen that for weak defect potentials the local density of states $A_\downarrow(\varepsilon)$ deviates only marginally from $N^0_\downarrow(\varepsilon)$.

For intermediate values of V, the bound states do not form, but a large reorganization of the density of states at the defect site takes place. It is worth pointing out that, in this region of V, even the largish value of W which we have used does not lead to appreciable changes of $A_\downarrow(\varepsilon)$ as compared to the $W = 0$ result.

Finally, for strong attractive defects with $|V| > |V_c|$, where $|V_c| \approx 0.489\Lambda$, a defect bound state forms below the unperturbed continuum, if $W = 0$. For finite interband coupling W,

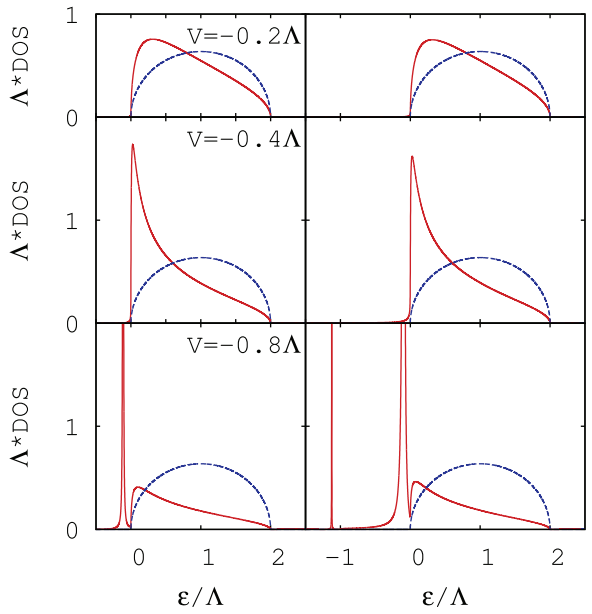

FIG. 2. (Color online) Local density of states of the minority band $A_\downarrow(\varepsilon)$ for $J = \Lambda$ and several values of V. Left column: $W = 0$. Right column: $W/V = 0.2$. In order to visualize the bound states, the energy ε has been given a small imaginary part $\gamma = 0.001\Lambda$.

the bound state turns into a Fano-type resonance because of its coupling to the continuum of majority-spin states. Moreover, in $A_\downarrow(\varepsilon)$ one can also observe a delta-function peak with a small weight, corresponding to the majority-band bound state.

B. Resistivity

In order to account for the nonperturbative effects found in the density of states, the resistivity will be calculated making use of Eq. (3), where the lifetime is determined from the optical theorem[27]

$$\frac{1}{\tau_\lambda} = -\frac{2n_{\rm imp}}{\hbar}\mathrm{Im}T_{\lambda\lambda}(\mu). \tag{5}$$

One can check readily that this expression reproduces Eq. (2) in the weak-scattering limit. In particular, also the interband scattering contributions to Eq. (2) are included in Eq. (5).

In Fig. 3 we plot the evolution, with decreasing exchange splitting J, of the matrix elements $-\mathrm{Im}T_{\lambda\lambda}(\mu)$ at the chemical potential for a realistic interband coupling $W/V = 0.05$ and several attractive defect potentials V in the vicinity of the critical coupling V_c for the bound-state formation. The majority-band matrix element $-\mathrm{Im}T_{\uparrow\uparrow}(\mu)$ is seen to be essentially constant for $J > J_c$ and it exhibits a sudden increase for $J < J_c$. The minority-band matrix element $-\mathrm{Im}T_{\downarrow\downarrow}(\mu)$ exhibits large structure when the chemical potential μ crosses the Fano resonances below the minority band and also when μ enters the minority band. The Fano resonances are reflected also in weak features of $-\mathrm{Im}T_{\uparrow\uparrow}(\mu)$.

In order to calculate the resistivity, we need an estimate of the effective mass. We shall take $m_\uparrow = m_\downarrow = m$, where

$$m = (4\pi)^{2/3}\frac{\hbar^2}{\Lambda a^2} \tag{6}$$

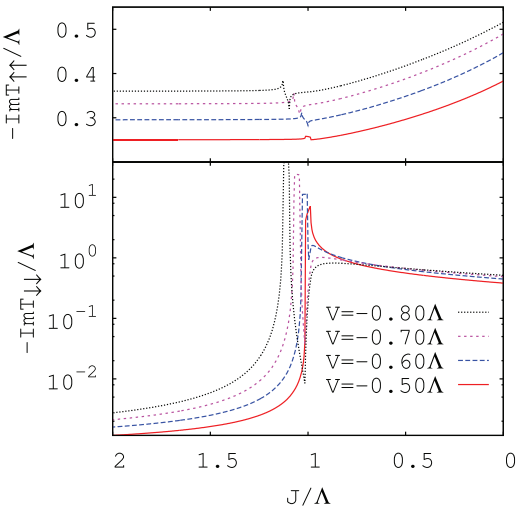

FIG. 3. (Color online) The matrix elements $-\mathrm{Im}T_{\lambda\lambda}(\mu)$ as functions of the exchange splitting J for $W/V = 0.05$ and several values of V. The upper panel and the lower panel (note the logarithmic scale) correspond to $-\mathrm{Im}T_{\uparrow\uparrow}(\mu)$ and $-\mathrm{Im}T_{\downarrow\downarrow}(\mu)$, respectively. The scale of J is chosen so that the applied pressure increases from left to right.

is the effective mass consistent with the postulated shape of the density of states at the band edges and a is the lattice constant, for which we take its zero-pressure value $a = 4.70$ Å. Plugging Eqs. (5) and (6) into Eq. (3), we find

$$\frac{1}{\rho_0} = \frac{e^2}{2(4\pi)^{2/3}\hbar a n_{\rm imp}}\sum_\lambda \frac{n_\lambda}{-\mathrm{Im}T_{\lambda\lambda}(\mu)/\Lambda}. \tag{7}$$

Making use of the results for $-\mathrm{Im}T_{\lambda\lambda}(\mu)$ in Eq. (7) we finally obtain the residual resistivity as a function of the exchange splitting J, see Fig. 4, which is the main result of this work. As is evident from Fig. 4, the residual resistivity ρ_0 is roughly constant at exchange splittings $J > J_c$ and for $J < J_c$ it exhibits a sharp increase. Moreover, for attractive defect potentials V strong enough to induce bound states below the minority band, there appears also a resonant-like anomaly of ρ_0 close to J_c. Thus we have qualitatively reproduced all the main features of the experimental data. It is also pleasing that the experimental magnitude of ρ_0 is reproduced for a reasonable concentration $n_{\rm imp} = 0.01$ of the typical defects.

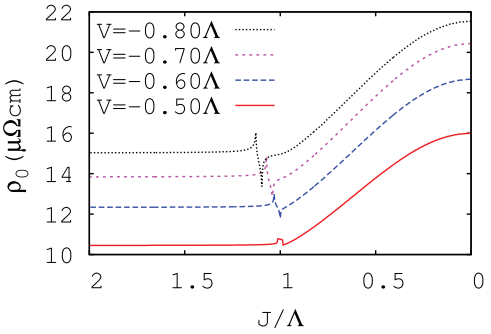

FIG. 4. (Color online) Residual resistivity ρ_0 as a function of the exchange splitting J for $W/V = 0.05$ and several values of V. For the concentration of point defects we take $n_{\rm imp} = 0.01$.

As regards the resonant peak in the vicinity of $J = J_c$, comparison of the data presented in Figs. 3 and 4 clearly shows that its physical origin lies in the scattering of the majority-spin electrons into the resonant states of the minority band. On the other hand, the smooth increase of ρ_0 for $J < J_c$ is caused by the decreasing number of the majority-spin electrons with high mobility at the expense of the minority-spin electrons with low mobility, as well as by the J dependence of $-\mathrm{Im}T_{\uparrow\uparrow}(\mu)$; see Fig. 3.

V. CONCLUSIONS

In this paper we have shown that even pure potential scattering is off-diagonal in the spin index in a helical ferromagnet such as FeGe. Building on this observation, within the standard transport theory we have calculated the evolution of the residual resistivity ρ_0 of a helical ferromagnet with changing exchange splitting J. We have assumed that the residual resistivity is dominated by scattering on a dilute gas of identical point defects. The scattering on a single point defect has been treated exactly. Sharp increase of ρ_0 has been found for the critical exchange splitting J_c where a locally fully polarized state turns into a partially polarized state. Furthermore we have shown that resonant-like anomalies of ρ_0 may appear in the vicinity of J_c, if the diagonal point defect potential is attractive and sufficiently strong.

Exactly this type of anomaly has been observed recently[16] in FeGe at a critical pressure $p_c \approx 19$ GPa. This leads us to conclude that the effect of pressure on FeGe can be modeled by a decrease of the exchange splitting until at p_c the minority spin Fermi sheet starts to become populated, resulting in a locally partially polarized state.

This work was motivated by the finding of intermediate partially polarized states in theoretical studies of several microscopic models of the isostructural and isoelectronic $FeSi_{1-x}Ge_x$ alloys,[17–20] as well as of FeGe under pressure[21,22] and of FeSi in applied magnetic fields.[23] We would like to emphasize, however, that our results should be quite independent of the details of the theoretical models and they should apply to any Lifshitz-type transition with a new Fermi surface sheet opening at the critical point, provided there exists a finite scattering amplitude between the bands.

In order to avoid misunderstandings, it should be pointed out that our calculation does not apply to the residual resistivity of the alloys $FeSi_{1-x}Ge_x$, which is a strongly disordered system with a high concentration of defects unless x is very close to 0 or 1. The picture presented here is falsifiable by magnetization measurements of FeGe under pressure. Let us note that by applying chemical pressure in the $FeSi_{1-x}Ge_x$ alloys, a weakly magnetic intermediate regime $0.25 < x < 0.4$ has in fact already been observed,[11] but we are not aware of any magnetization data for FeGe under pressure. Furthermore, if the analogy between FeGe under pressure and the $FeSi_{1-x}Ge_x$ alloys is sound, then we would expect a second phase transition in FeGe to an insulating state at a higher pressure p_c'. The authors of Ref. 21 estimate that this should happen at $p_c' \approx 40$ GPa.

Finally, our picture can also be falsified by measuring the pressure dependence of the total density of states at the Fermi level $N(\mu) = \sum_{\lambda=1,2} N_\lambda(\mu)$, which should exhibit an additional increase on top of a smooth change in the vicinity of $p = p_c$. By applying chemical pressure in the $FeSi_{1-x}Ge_x$ alloys, the density of states has already been determined from an analysis of the specific-heat data.[11] In the intermediate composition range $0.25 < x < 0.6$ an increased value of $N(\mu)$ has in fact been found, the enhancement with respect to the large-x samples reaching values up to $\approx$2.3. In order to be able to describe such large enhancements, most likely we will have to take into account that fully polarized states are uncorrelated within the Hubbard model, whereas partially polarized states do experience mass enhancement due to correlations. The studies of the density of states and of the finite-temperature resistivity are therefore genuine many-body problems and as such they are left for future work.

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