Theory of spin-fluctuation resistivity near the critical point of ferromagnets*

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A simple theory of electrical resistivity due to critical spin fluctuations $R_s(T)$ is presented in a form which is valid for ferromagnets with anisotropic Fermi surfaces. Subject to reasonable restrictions on the electronic band structure, it is shown that $dR_s(T)/dT$ is positive and proportional to the magnetic specific heat, in the $T\rightarrow T_c^+$ limit, for all ferromagnets which can be described by a spin Hamiltonian with only short-range forces. A detailed treatment is given of the temperature range above T_c where short-range ($R \ll \xi$) correlations no longer describe the spin fluctuations relevant to the resistivity problem. The gradual cross over to a regime dominated by longer-range correlations and the corresponding possibility of a change in sign of $dR_s(T)/dT$ at $T > T_c$ are studied and numerical results are given. The results are interpreted in terms of the structure of the spin correlation function $\Gamma(\vec{q}, T)$ and the Fermi-surface geometry and provide a unified interpretation of available experimental results.

I. INTRODUCTION

The study of transport properties at magnetic phase transitions, and of the electrical resistivity in particular, has received a good deal of attention. For a survey of the experimental results and for references to the original literature, we refer the reader to recent review articles.[1-3] There are still several questions which have not yet been satisfactorily answered. The objective of this work has been the generalization or extension of earlier theoretical results[4-6] so as to obtain a coherent and unified description of the different types of singularities or "anomalies" in the temperature derivative $\rho'(T)$ of the electrical resistivity at the Curie temperature T_C of ferromagnets. For present purposes,[7] we may distinguish three types of behavior of $\rho'(T)$ near T_C. These different forms exhibited by $\rho'(T)$ are illustrated schematically in Fig. 1. It should be pointed out that this classification of behavior is based on operational convenience and need not imply fundamental distinctions. Assuming Matthiessen's rule to provide an adequate approximation, the total resistivity is the sum of a spin-fluctuation component $\rho_s(T)$, a phonon component $\rho_{\text{ph}}(T)$, and a contribution due to static imperfections and lattice defects ρ_D. Taking the slowly varying phonon background into account, it is seen from Fig. 1 that nickel-like (type-I) ferromagnets have $\rho_s'(T)>0$ for both $T<T_C$ and $T>T_C$ throughout the entire observed critical range. In contrast, the intermetallic compound $GdNi_2$, which is taken to be the prototype of type-II ferromagnets, has $\rho_s'(T)>0$ for $T<T_C$ and for a short temperature

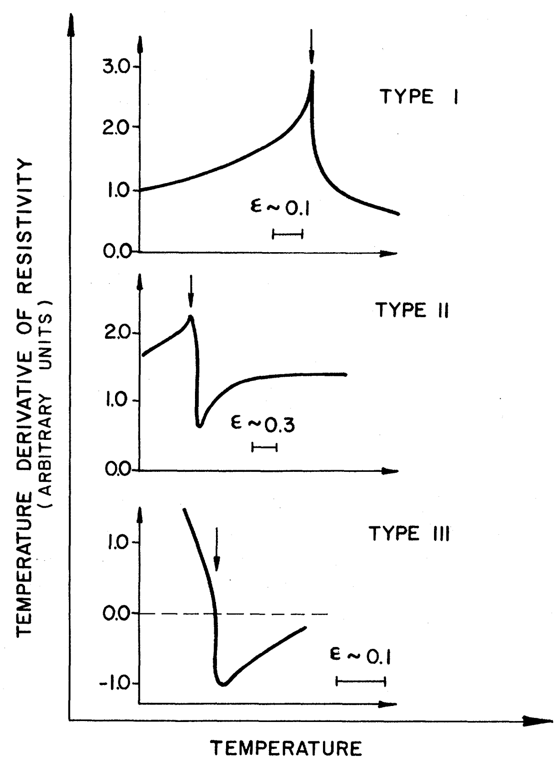

FIG. 1. Temperature derivative of resistivity vs temperature for type-I, -II, and -III behavior near the Curie temperature (indicated by an arrow). Reduced temperature scale, as indicated by ϵ, refers to the prototypes discussed in the text. Note that the phonon background contributes positive slope which must be subtracted in deducing the spin component from the total resistivity.

interval above T_C; $\rho_s'(T)$ changes sign and is negative in most of the paramagnetic state. The resistivity measured along the c axis of the rare-earth metal gadolinium, which is the prototype and perhaps the unique example of type-III ferromagnets, is different again. The *immediate vicinity* of T_C is a bit unclear owing to the extremely rapid variation of $\rho_s'(T)$. However, with this possible reservation, $\rho_s'(T)>0$ for $T<T_C$ but $\rho_s'(T)<0$ for the entire observed temperature range in the paramagnetic state.

Theory and experiment are in good qualitative agreement for type-I ferromagnets. By including short-range correlations in the de Gennes–Friedel[4] model, Fisher and Langer[5] showed that $\rho_s'(T)$ should vary as the magnetic specific heat C_m for $T\to T_C^+$. These results were extended by Richard and Geldart[6] (to be referred to as RG), who showed that $\rho_s'(T)\sim C_m$ for $T\to T_C^-$ as well. RG also showed that a consistent treatment of spin correlations in an Ornstein-Zernike approximation could lead to $\rho_s'(T)>0$ in the paramagnetic range, and they discussed the possibility of a transition from short-range dominance at T_C^+ to long-range dominance at higher temperature.

In Secs. II–IV, we extend the simple theory of resistance due to critical spin fluctuations to apply, as far as possible, to type-II and -III ferromagnets. Subject to reasonable conditions on the electronic band structure, it is proved analytically that short-range spin fluctuations always lead to $\rho_s'(T)>0$ at T_C^+. The possibility of a crossover to long-range dominance, described by a consistent Ornstein-Zernike regime, is discussed in detail. Special features introduced by small Fermi-surface calipers and by anisotropic Fermi surfaces are emphasized. Numerical results are given. Section V consists of a summary of results, discussion of the applicability of the model results to real systems, and some additional observations concerning the resistivity in the ordered state.

II. RESISTIVITY IN s-f EXCHANGE MODEL

The electrical resistivity due to spin fluctuations is due to electrons (labeled by wave number, band, and spin-projection-state indices $\vec{k}n\nu$) being scattered by spins $\vec{S}_l$ which are taken to be localized at lattice points $\vec{R}_l$. The (weak) coupling between the conduction electrons and the localized spins is of short-range s-f exchange origin.[4] To adequately discuss type-II and -III ferromagnets, we require a formulation of the resistivity problem which is valid for non-free-electron band structure. Useful solutions of the Boltzmann equation are not available in such cases, so we shall rely on the variational principle, according to which the resistivity in the ith crystal direction satisfies

$$\rho_S^i\le\rho_S^i(\phi)=\frac{1}{2k_BT}\,\frac{\sum_{\vec{k}n\nu}\sum_{\vec{k}'n'\nu'}Q_{\vec{k}'n'\nu',\vec{k}n\nu}f_{\vec{k}n\nu}(1-f_{\vec{k}'n'\nu'})(\phi_{\vec{k}n\nu}-\phi_{\vec{k}'n'\nu'})^2}{\left(e\sum_{\vec{k}n\nu}\phi_{\vec{k}n\nu}v^i_{\vec{k}n\nu}\dfrac{\partial f_{\vec{k}n\nu}}{\partial\epsilon_{\vec{k}n\nu}}\right)^2}\,, \tag{1}$$

with the equality holding when $\phi_{\vec{k}n\nu}$ corresponds to the exact solution to the Boltzmann equation.[8] In Eq. (1), k_B is the Boltzmann constant, T is the absolute temperature, e is the electron charge, $f_{\vec{k}n\nu}$ is the Fermi function, $\epsilon_{\vec{k}n\nu}$ is the electron energy, and $v^i_{\vec{k}n\nu}$ is the ith component of the electron velocity $\nabla_{\vec{k}}\epsilon_{\vec{k}n\nu}/\hbar$. The transition rate for electron scattering in the second Born approximation is given, in the paramagnetic state, by

$$Q_{\vec{k}n\nu,\vec{k}'n'\nu'}=\frac{\Omega_0}{\hbar^2}|M_{\vec{k}'n'\nu',\vec{k}n\nu}|^2\sum_{\vec{R}}\exp[-i(\vec{k}-\vec{k}')\cdot\vec{R}]\int_{-\infty}^{\infty}dt\exp[i(\epsilon_{\vec{k}n\nu}-\epsilon_{\vec{k}'n'\nu'})t/\hbar]\langle(\vec{\sigma}_{\nu'\nu}\cdot S_{\vec{0}})[\vec{\sigma}_{\nu\nu'}\cdot\vec{S}_{\vec{R}}(t)]\rangle\,, \tag{2}$$

where Ω_0 is the volume per ion, M denotes a matrix element of the s-f exchange interaction, $\vec{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ are the Pauli matrices, and $\vec{S}_{\vec{R}}(t)$ has the time dependence of the Heisenberg picture.

The utility of the variational formulation obviously lies in the fact that simple "approximate" forms for $\phi_{\vec{k}n\nu}$ may be used in Eq. (1), which, being stationary for the "exact" $\phi_{\vec{k}n\nu}$, then yields an estimate of ρ_s^i. An exact solution in simple isotropic cases and a physically reasonable approximation in anisotropic cases is given by $\phi_{\vec{k}n\nu}=v^i_{\vec{k}n\nu}$; this will be used exclusively in the following.[9] Near the critical temperature the spin-fluctuation lifetime is sufficiently long that the scattering is quasielastic. The time dependence of $\vec{S}_{\vec{R}}(t)$ may then be neglected. The time integral in Eq. (2) then yields the usual energy-conserving δ function. As a further simplification, matrix elements of the short-range exchange interaction are replaced by a suitable average value $|M|^2$. Putting all of these results into Eq. (1),

$$\rho_s^i(T) = \sum_{\vec{R}} \langle \vec{S}_{\vec{0}} \cdot \vec{S}_{\vec{R}} \rangle G^i(\vec{R}T) \,, \tag{3}$$

where

$$G^i(\vec{R}T) = \frac{2\pi\Omega_0|M|^2}{2k_BT\hbar} \, \frac{\sum_{\vec{k}n}\sum_{\vec{k}'n'} e^{-i(\vec{k}-\vec{k}')\cdot\vec{R}} f_{\vec{k}n}(1-f_{\vec{k}'n'})\delta(\epsilon_{\vec{k}n}-\epsilon_{\vec{k}'n'})(v^i_{\vec{k}n}-v^i_{\vec{k}'n'})^2}{\left(2e^2\sum_{\vec{k}n}(v^i_{\vec{k}n})^2\frac{\partial f_{\vec{k}n}}{\partial \epsilon_{\vec{k}n}}\right)^2} \,. \tag{4}$$

Low-temperature approximations are valid for the Fermi functions since $k_BT_C \ll \epsilon_F$, the Fermi energy. It is convenient to normalize the resistivity to its high-temperature limit, $\rho^i_{0s} = \rho^i_s(T \gg T_C)$. Introducing

$$\Gamma(\vec{R}T) = \langle \vec{S}_{\vec{0}} \cdot \vec{S}_{\vec{R}} \rangle / S(S+1) \,, \tag{5}$$

Eq. (3) becomes

$$R^i_s(T) = \rho^i_s(T)/\rho^i_{0s} = \sum_{\vec{R}} \Gamma(\vec{R}T)\Phi^i(\vec{R}) \,, \tag{6}$$

with

$$\Phi^i(\vec{R}) = \frac{\sum_{\vec{k}n}\sum_{\vec{k}'n'} e^{-i(\vec{k}-\vec{k}')\cdot\vec{R}} \delta(\epsilon_{\vec{k}n}-\epsilon_F)\delta(\epsilon_{\vec{k}'n'}-\epsilon_F)(v^i_{\vec{k}n}-v^i_{\vec{k}'n'})^2}{\sum_{\vec{k}n}\sum_{\vec{k}'n'} \delta(\epsilon_{\vec{k}n}-\epsilon_F)\delta(\epsilon_{\vec{k}'n'}-\epsilon_F)(v^i_{\vec{k}n}-v^i_{\vec{k}'n'})^2} \,. \tag{7}$$

It should be emphasized that these results are valid for arbitrary nondegenerate band structures and that the electron energies and velocities which enter have the correct lattice periodicity when translated by any reciprocal lattice vector. It is then clear from Eq. (7) that

$$\sum_{\vec{R}} \Phi^i(\vec{R}) = 0 \,. \tag{8}$$

This sum rule was discussed by RG and has the physical consequence that a periodic potential, considered as a possible scattering mechanism, yields zero resistance. Equation (8) will be important in later discussion. Since this result was derived assuming a sharply defined Fermi surface (which does not always exist due to disorder in the system), it is reasonable to ask whether Eq. (8) still holds when the finite electron mean free path is taken into account. For simplicity, consider a single-band model and assume that the finite electron lifetime $\tau = h/\Gamma$ can be described in a Breit-Wigner approximation, so that an additional factor of $e^{-|t|/\tau}$ appears in Eq. (2). Then the δ function in Eq. (4) is replaced by $(\Gamma/\pi)[(\epsilon_{\vec{k}n}-\epsilon_{\vec{k}n''})^2+\Gamma^2]^{-1}$, which is always finite. The velocity transfer factors in Eqs. (4) and (7) are assumed not to be "smeared out" by the disorder, so that Eq. (8) still results.

Upon some reflection, it is seen that this situation also persists even when multiple bands and interband transitions are included, provided the thermal (k_BT) and disorder (Γ) smearing of the Fermi surface can be neglected in comparison to the excitation energies to the first normally unpopulated band. Thus, to this level of approximation, Eq. (8) may be considered to be of general validity.

In obtaining estimates for $R^i_s(T)$, it is often convenient to use a free-electron model to describe $\Phi^i(\vec{R})$, or its corresponding Fourier integral transform

$$\Phi^i(\vec{q}) = \int d^3r\, \Phi^i(\vec{r})\, e^{-i\vec{q}\cdot\vec{r}} \,. \tag{9}$$

For free electrons, the integrals in Eq. (7) are elementary, and Eq. (9) yields

$$\Phi^i(\vec{q}) = (3\pi^2/2k_F^4)(q_i^2/q)\Theta(2k_F - q) \,, \tag{10}$$

where q_i is the component of $\vec{q}$ in the direction of the applied field and $\Theta(x)$ is the usual unit step function. In the case where disorder smearing of the electron energy is explicitly included in a Breit-Wigner approximation (as discussed above), Eq. (10) can be shown to be modified by an additional factor of $4q\epsilon_F/\pi k_F\Gamma$ in the $q \ll 1/l$ limit, where l is the electron mean free path. This will be commented upon in the Sec. III.

In the case of type-III ferromagnets, we shall consider a model in which the electron (hole) dispersion law is anisotropic, having only cylindrical symmetry, and is of the form

$$\epsilon_{\vec{k}} = \pm\hbar^2[k_z^2/2m_c + (k_x^2+k_y^2)/2m_a] + \text{const}, \tag{11}$$

where the + (−) sign refers to electron (hole) excitations. $\Phi^i(\vec{q})$ can still be explicitly evaluated in this model. From Eqs. (7) and (9), we require

$$\Phi^i(\vec{q}) = \frac{\int d^3k\, \delta(\epsilon_{\vec{k}} - \epsilon_F)\delta(\epsilon_{\vec{k}+\vec{q}} - \epsilon_F)(v^i_{\vec{k}} - v^i_{\vec{k}+q})^2}{\int d^3k\, d^3k'\, \delta(\epsilon_{\vec{k}} - \epsilon_F)\delta(\epsilon_{\vec{k}'} - \epsilon_F)(v^i_{\vec{k}} - v^i_{\vec{k}'})^2} \,. \tag{12}$$

Changing variables by $k^j \to (\sqrt{m^j})k^j$, etc., the integration in Eq. (12) is reduced to the previous isotropic case and we obtain

$$\Phi^i(\vec{q}) = \frac{3\pi^2 q_i^2}{2k_{Fc}^2 k_{Fa}^2}\, \frac{m_c/m^i}{q^*}\, \Theta(2k_{Fc} - q^*)\,, \tag{13}$$

where k_{Fc} (k_{Fa}) is half the Fermi-surface caliper in the c (a) direction and

$$q^* = [q_z^2 + (q_x^2 + q_y^2)m_c/m_a]^{1/2}\,.$$

On the basis of these simple models for the electron dispersion law and Fermi surface, Secs. III and IV deal with how different types of spin correlation functions yield characteristic resistive anomalies.

Various forms can be written for the resistivity; for example, if a Fourier representation is used for the functions in Eq. (6), we have

$$R_S^i(T) = \int \frac{d^3\vec{q}}{(2\pi)^3}\, \Phi^i(\vec{q})\Gamma_L(-\vec{q}, T)\,, \tag{14}$$

where the integration is over all $\vec{q}$ space. The Fourier lattice transforms are defined by

$$F_L(\vec{q}, T) = \sum_{\vec{R}} e^{-i\vec{q}\cdot\vec{R}} F(\vec{R}, T)\,,$$

and are related to Fourier integral transforms by

$$F_L(\vec{q}, T) = \frac{(2\pi)^3}{\Omega_0} \sum_{\vec{G}} F_I(\vec{q} + \vec{G}, T)\,, \tag{15}$$

where the last sum is over all reciprocal-lattice vectors (including zero). For simplicity, we have neglected the minor complications which are required in the case of a non-Bravais lattice.

III. SPIN-FLUCTUATION RESISTIVITY FOR $T \to T_C^+$

It was noted by Fisher and Langer[5] that the lattice sum in Eq. (6) has an inherent cutoff R_c (which may be the finite electron mean free path or another relevant electronic length scale), so that the dominant contributions to $R_S^i(T)$ come from terms in the sum for which $|\vec{R}| \lesssim R_c$. However, the length scale of the spin correlation function is $\xi(T) = \xi_0 \epsilon^{-\nu}$, which increases indefinitely as

$$\epsilon = (T - T_C)/T_C \to 0$$

(standard notation for critical indices will be used[10]). Consequently, the form of the correlation function used in Eq. (6) must be that appropriate to the limit $R \lesssim R_c \ll \xi$ when T is sufficiently close to T_C. The effective spin-spin interaction, which determines the magnetic internal energy and the critical specific heat $C \sim \epsilon^{-\alpha}$, is assumed to be of a reasonably short-range Heisenberg form. In order to be consistent with the specific heat, the spin correlation function must be

$$\Gamma(RT) = D(\kappa R)/(R/a)\,,$$

where $\kappa = 1/\xi$, a is the lattice constant, and $D(\kappa R)$ is given for $\kappa R \ll 1$ by[11]

$$D(x) = D_0 - D_1 x^{(1-\alpha)/\nu} - D_2 x^{1/\nu} - \cdots\,. \tag{16}$$

Of course, precisely this same $\Gamma(RT)$ determines the electrical resistivity due to critical spin fluctuations, so we have

$$\delta R_S^i(T) = R_S^i(T) - R_S^i(T_C) = A^i \epsilon^{1-\alpha} + B^i \epsilon + \cdots\,, \tag{17}$$

where

$$A^i = -D_1(\kappa_0 a)^{(1-\alpha)/\nu} \sum_{\vec{R}} (R/a)^{\phi}\Phi^i(R) \tag{18}$$

and

$$\phi = (1-\alpha)/\nu - (1+\eta)\,.$$

B^i is given by a similar form in which $\alpha \to 0$.

It was an approximate version of Eq. (18) which was evaluated by Fisher and Langer,[5] who concluded that $A^i > 0$ and hence $\rho'(T) > 0$ near T_C for type-I ferromagnets. The work of RG, who evaluated Eq. (18) by numerical methods, was restricted to a free-electron model. We now extend these results by giving a simple analytical demonstration that A^i and $d\rho^i/dT$ are positive for $T \to T_C^+$ for arbitrary nondegenerate band structure.

Since the contributions to the sum in Eq. (6) come from $R \lesssim R_c$, it is clear that the sum will be virtually unchanged by introducing an additional factor $e^{-\lambda R}$, provided that $\lambda \ll 1/R_c$ and that there is no change at all if the $\lambda \to 0$ limit is taken at some appropriate point. However, this device serves to define the Fourier transform of

$$\delta\Gamma^\lambda(RT) = [\Gamma(RT) - \Gamma(RT_C)]\, e^{-\lambda R}. \tag{19}$$

Explicitly, the Fourier integral transform is

$$\delta\Gamma_I^\lambda(qT) = -\frac{4\pi D_1(\kappa a)^{(1-\alpha)/\nu}\,\Gamma(2+\phi)\sin[(2+\phi)\tan^{-1}(q/\lambda)]}{a^{\phi} q (q^2 + \lambda^2)^{1+\phi/2}}\,. \tag{20}$$

For the commonly occurring critical exponents, $0 < \phi < 1$ (in fact, $\phi \lesssim \frac{1}{2}$), so it is seen from Eq. (20) that $\delta\Gamma_I^\lambda(qT)$ is positive for $q > \lambda_0$ and is negative for $q < \lambda_0$, where $\lambda_0 = \lambda \tan[\pi/(2+\phi)]$. These negative contributions may be isolated by writing Eq. (17) as

$$\delta R_S^i(T) = \int \frac{d^3q}{(2\pi)^3}\, \Phi_I^i(\vec{q})\delta\Gamma_L^\lambda(\vec{q}T)\,. \tag{21}$$

Note from Eqs. (7) and (9) that $\Phi_I^i(\vec{q}) \geq 0$ and that $\Phi_I^i(\vec{q})$ vanishes (at least linearly) when $\vec{q} \to \vec{0}$. Also, because of the Bloch periodicity of the velocities in Eq. (7), $\Phi_I^i(\vec{q}) \to 0$ when $\vec{q} \to \vec{G}$, where $\vec{G}$ is a reciprocal-lattice vector. From Eqs. (15) and (20), $\delta\Gamma_L^\lambda(\vec{q}T)$ is negative for $|\vec{q}-\vec{G}| < \lambda_0$, where $\vec{G}$ is any reciprocal-lattice vector (including zero).

First consider the negative contribution to Eq. (21) from $q < \lambda_0$. From Eq. (20), it is easy to place upper and lower bounds on $\delta\Gamma_I^\lambda(qT)$ in this region, so that the magnitude of the corresponding contribution to Eq. (21) is of order

$$\epsilon^{1-\alpha}\int_0^{\lambda_0} dq\, \frac{q^2\Phi_I^i(\vec{q})}{q^{3+\phi}} \propto \lambda^{1-\phi}\,,$$

if the finite electron mean free path is neglected. If the finite mean free path is retained as in Sec. II, $\Phi_I^i(\vec{q}) \propto q^2$ for $q \to 0$, so $\lambda^{2-\phi}$ results. The corresponding negative contributions to Eq. (21) from the regions where $|\vec{q}-\vec{G}| < \lambda_0$ are also of order

$$\epsilon^{1-\alpha}\int_{|\vec{q}-\vec{G}|<\lambda_0} d^3q\, \frac{\Phi_I^i(\vec{q})}{|\vec{q}-\vec{G}|^2} \propto \lambda^{1-\phi}\,,$$

since $\Phi_I^i(\vec{q})$ vanishes (at least linearly) for $\vec{q} \to \vec{G}$. We conclude that all negative contributions can be isolated and that the $\lambda \to 0$ limit can be taken (just as in the original $\vec{R}$-space sums) and that only *positive* contributions to $\delta R_S^i(T)$ remain.

The conclusion that $\delta R_S^i(T) > 0$, so that

$$\frac{\partial R_S^i}{\partial T} > 0$$

for $T \to T_C^+$, is valid for a wide class of band structures as described in Sec. II. The specific prediction of the T dependence,

$$\frac{\partial R_S^i}{\partial T} \propto C_S\,,$$

followed from the scaling form of Eqs. (15) and (16). However, the conclusion that $\delta R_S^i(T) > 0$ for $T \to T_C^+$ would follow for a wide class of functions $\Gamma(RT)$, subject to being appropriately decreasing functions of both R and T, is insensitive to moderate deviations from strong scaling. These results are all valid in the strict limit of $T \to T_C^+$. For finite values of ϵ, higher-order terms in the expansion of Eq. (16) become important, and the possibility that the short-range expansion may break down and that $\delta R_S^i(T)$ may change sign cannot be excluded. This is discussed in Sec. IV.

IV. SPIN-FLUCTUATION RESISTIVITY FOR $T > T_C$

The results of Sec. III are, strictly speaking, limited to the $T \to T_C^+$ limit, since the short-range expansion, Eq. (16), for $D(x)$ must fail for values of $x = \kappa R$ somewhat less than unity. Thus an alternative form for $\Gamma(RT)$ must be found which is valid for $\kappa R \gtrsim 1$. One such approximation, suggested by Ferer, Moore, and Wortis,[12] is of modified Ornstein-Zernike (OZ) form

$$\Gamma(\vec{R}T) = \begin{cases} 1\,, & R = 0\,, \\ C(\kappa a)^\eta \dfrac{e^{-\kappa R}}{R/a}\,, & R \geq a\,, \end{cases} \tag{22}$$

which was estimated, on the basis of numerical analysis of Ising-model data, to be valid for $\kappa a > 0.1$. A simpler approximation of OZ form was introduced by RG:

$$\Gamma^{OZ}(\vec{R}T) = \begin{cases} 1\,, & R = 0\,, \\ C\dfrac{e^{-\kappa R}}{R/a}\,, & R \geq a\,, \end{cases} \tag{23}$$

where the constant $C \approx 0.2$ is taken to fit the nearest-neighbor correlations near T_C. This approximation satisfies two major requirements for a physically correct correlation function for simple ferromagnets: (a) $\Gamma(\vec{R},T) = 1$ at $\vec{R} = \vec{0}$ for *all* T, and (b) $\Gamma(RT)$ is a decreasing function of both R and T for $R \neq 0$. It was shown by RG that the Fourier lattice transform of Eq. (23), $\Gamma_L^{OZ}(\vec{q},T)$, qualitatively resembles the *exact* correlation function.[5] In particular, $d\Gamma_L^{OZ}(\vec{q},T)/dT$ is positive for $\kappa \ll q$ and negative for $q \ll \kappa$, so that at fixed $\vec{q}$, $\Gamma_L^{OZ}(\vec{q},T)$ has a maximum as a function of T at $T_0(\vec{q}) > T_C$. Consequently, Eq. (23) describes not only the long-range ($\kappa R > 1$) regime but also qualitatively describes the gross features (although not the precise temperature dependence, of course) of correlations closer to T_C.

Using $\Gamma^{OZ}(\vec{R},T)$, it is very simple to calculate the contribution of spin fluctuations to physical properties of the system. Consider first the electrical resistivity. From Eqs. (6) and (23),

$$R_S^i(T) = 1 + \sum_{\vec{R}\neq\vec{0}} \Phi^i(\vec{R})\frac{Cae^{-\kappa R}}{R}\,, \tag{24}$$

so

$$\frac{\partial R_S^i(T)}{\partial \kappa} = -Ca\sum_{\vec{R}\neq 0} \Phi^i(\vec{R})e^{-\kappa R}\,. \tag{25}$$

For $\kappa \to 0$, the right-hand side is just

$$Ca\Big(1 - \sum_{\vec{R}} \Phi^i(\vec{R})\Big) = Ca$$

from Eq. (8). Thus, a treatment of correlations in a *consistent* OZ approximation also yields

$$\frac{\partial R_S^i(T)}{\partial T} > 0$$

near T_C, in agreement with the treatment in Sec. III. The corresponding calculation of the heat capacity is also elementary. Assuming a Heisenberg model for the spin-spin interaction, the specific heat per spin is

$$\frac{C_S(T)}{N} = -\frac{d}{dT}\sum_{\vec{R}\neq\vec{0}} J(\vec{R})S(S+1)\frac{Cae^{-\kappa R}}{R}$$

$$\to Ca\kappa'(T)S(S+1)\sum_{\vec{R}\neq\vec{0}} J(\vec{R})$$

$$= Ca\kappa'(T)(\tfrac{3}{2}T_{C0}), \qquad (26)$$

where T_{C0} is the mean-field approximation to the critical temperature. Thus $\partial R_S^i(T)/\partial T$ and $C_S(T)/N$ are found to have the same temperature dependence near T_C and their ratio is $2/(3T_{C0})$, just as was found by Mannari[13] via a very different approach.

These results strongly suggest that the consistent OZ approximation, Eq. (23), may be quite adequate to discuss the crossover from short-range dominance near T_C^+ to long-range dominance at higher temperatures. The importance of doing so within a unified, albeit approximate, theory should not be underestimated.

Before continuing, it is necessary to be more precise about the cutoff R_c which enters into the electronic factor $\Phi(\vec{R})$ in Eq. (24). It has already been indicated[5] that the finite electron mean free path l is a possible cutoff. However, subject to a sufficiently sharp Fermi surface, $\Phi^i(\vec{R})$ contains oscillatory factors (e.g., $\cos 2k_F R$ in the case of an isotropic Fermi surface) which are equally effective as cutoffs, so that $(2k_F)^{-1}$ is also a possible cutoff. For any metals to which the theory of Sec. II may reasonably be expected to apply, it is necessary that disorder smearing of the Fermi surface be relatively unimportant, i.e., $1/l$ must be somewhat less than $2k_F$. In this case, the effective cutoff of $\vec{R}$-space sums is the inverse Fermi-surface caliper, and the dominant contributions to the resistivity come from transitions with

$$|\vec{k}-\vec{k}'| = q \lesssim 1/R_c = 2k_F,$$

in agreement with the conclusion of Fisher and Langer[5]; the electron mean free path plays no essential role.

The above considerations suggest that $\kappa(T)/2k_F$ is a relevant parameter to characterize the possible sign change of $dR_S^i(T)/dT$ and the crossover from short-range to long-range dominance. It is thus necessary to estimate, albeit very roughly, the value of k_F appropriate to the metals which we are attempting to describe. The band structure of magnetic metals is rather complex, of course. The simplest model which we may reasonably adopt in the case of basically cubic metals, such as fcc Ni (type-I) and cubic Laves phase $GdNi_2$ (type-II), is that the dominant current carriers are associated with isotropic (electron or hole) pockets of *sp* character. The Fermi-surface caliper $2k_F$ of such pockets is expected to be somewhat less than the dimension $\sim 2\pi/a$, of the first Brillouin zone. Values of $2k_F/(2\pi/a)$ in the range 0.1–0.5 are not unreasonable. Type-III ferromagnets will be discussed later.

Having decided upon the relevant model parameters, the slope of the resistivity is given by Eq. (25), which can be rewritten

$$\frac{dR_S^i(T)}{d\epsilon} = \frac{Ca\nu\kappa}{\epsilon}S^i(\kappa), \qquad (27)$$

with

$$S^i(\kappa) = 1 - \sum_{\vec{R}} \Phi^i(\vec{R})e^{-\kappa R}$$

$$= 1 - \frac{1}{\Omega_0}\sum_{\vec{G}}\frac{d^3\vec{q}}{(2\pi)^3}\frac{8\pi\kappa}{|(\vec{q}+\vec{G})^2+\kappa^2|^2}\Phi_I^i(\vec{q}). \qquad (28)$$

Note that all terms in the sum over reciprocal-lattice vectors are positive and tend to reduce the slope of the resistivity from its value near T_C. In the range of present interest, κ and $2k_F$ are both significantly less than $2\pi/a$, so the sum in Eq. (28) converges rapidly and is dominated by the $\vec{G}=\vec{0}$ term.[14] Using Eq. (10) and averaging over the three equivalent crystal directions, the integral in Eq. (28) is easily evaluated to give

$$S(\kappa) = \frac{1}{3}\sum_i S^i(T)$$

$$= 1 - \frac{2}{\pi^2 d^3}\left[\beta\ln\left(\frac{1+\beta^2}{\beta^2}\right) - \frac{\beta}{1+\beta^2}\right], \qquad (29)$$

where $d = k_F a/\pi$ and $\beta = \kappa/2k_F$. In Fig. 2, we have plotted

$$\frac{dR_S(T)}{d\epsilon} = \sum_i \frac{1}{3}\frac{dR_S^i(T)}{d\epsilon}$$

as a function of $\log_{10}\epsilon$, for a range of values of d.

First consider the case of type-I ferromagnets, which have high values of T_C. It is clear that the positive slope of $R_S(T)$ observed for these systems in the paramagnetic range[2,3] is consistent with Fig. 2, provided the substantial *sp* pockets of current carriers have Fermi-surface calipers $2k_F$ which satisfy $d = k_F a/\pi > d_0 \approx 0.6$. On the other hand, type-II ferromagnets have considerably lower transition temperatures (e.g., T_C for $GdNi_2$ is an order of magnitude smaller than that for Ni). The fact that their resistivity curves exhibit more structure than do type-I ferromagnets over the same range of ϵ suggests, on the basis of Fig. 2,

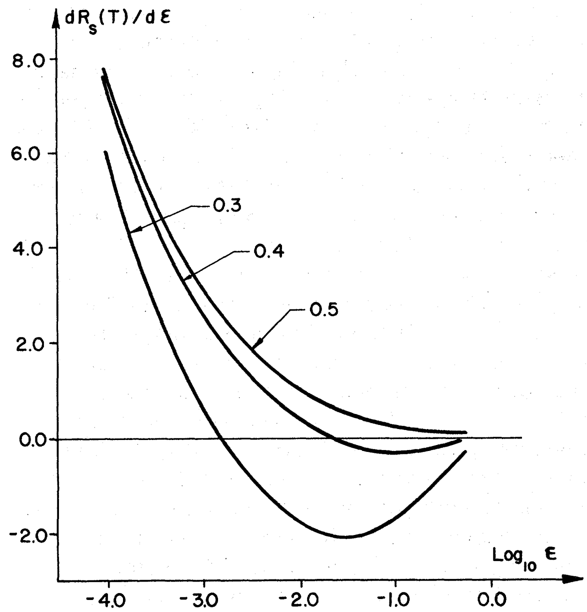

FIG. 2. Reduced temperature derivative of resistivity vs the logarithm of reduced temperature for the isotropic model. Each curve is labeled by the corresponding value of $2k_F/(2\pi/a)$, i.e., 0.3, 0.4, and 0.5.

that the dominant current carriers in type-II ferromagnets are to be associated with correspondingly smaller Fermi-surface pockets. This suggestion is consistent with the relatively low transition temperatures for such systems in which the dominant magnetic interaction between the localized rare-earth ions is of indirect exchange origin.

We conclude that both type-I and type-II ferromagnets can be adequately accounted for by the present description. The substantial differences observed in their resistivities are ascribed to Fermi-surface characteristics rather than to qualitative differences of a fundamental nature. In either case, of course, $dR_S(T)/dT > 0$ varies as the magnetic specific heat for T sufficiently close to T_C. Reliable estimates of the temperature range of validity of the corresponding power law are not possible without adequate knowledge of the higher-order terms in the expansion for $D(\kappa R)$ in Eq. (16). This point will not be pursued here; it is sufficient to note that the short-range expansion is certainly invalid in the temperature range where $dR_S(T)/dT$ changes sign.

The case of type-III ferromagnets is particularly intriguing for several reasons, among which are the following: The resistivity of Gd is highly anisotropic; when measured with the current flowing along the c axis of the hcp crystal, $R^c(T)$ clearly has *negative* slope for $T \gtrsim T_C$ and throughout the observed paramagnetic range. This fact has to be reconciled with the conclusions of Sec. III and will be returned to subsequently. However, the resistivity of Gd with the current flowing in the basal plane, $R^b(T)$, has *positive* slope and, generally speaking, has roughly the form characteristic of type-I ferromagnets. Our first task will be to show how $dR^c(T)/dT < 0$ with $dR^b(T)/dT > 0$ at the same temperature can be consistently obtained in the paramagnetic state. From the previous results for isotropic systems, it is clear that the Fermi-surface geometry may play an important role.

The Fermi surface of Gd is known from band-structure calculations to be highly anisotropic; for details we refer the reader to a recent review by Freeman.[15] The only portions of the calculated (hole) Fermi surface which have significant velocity components parallel to the c axis of the hcp Brillouin zone are found in the network of arms located near the hexagonal faces of the zone.[15] The Fermi-surface caliper in the c axis direction of these arms is rather small, but the average caliper in the basal plane is somewhat larger. Relative to the appropriate reciprocal-lattice vectors, $2k_{Fc} \approx 0.2(2\pi/c)$ while $2k_{Fb} \approx 0.4(4\pi/\sqrt{3}a)$, where c and a denote the usual lattice constants.

We believe that the above features of the Fermi surface of Gd play an important role in determining the resistivity, and accordingly have adopted the following simple model to illustrate the point: Portions of the Fermi surface having their velocity vectors largely perpendicular to the c axis of the zone are ignored totally, and the network of arms is replaced by a single ellipsoid having cylinder symmetry about the c axis. The Fermi-surface calipers of this ellipsoid are taken to be $2k_{Fc}$ and $2k_{Fb}$, as given above, for the c and basal-plane axes, respectively. The dispersion law for this model has already been stated in Eq. (11), and the corresponding anisotropic $\Phi_I^i(\vec{q})$, which is given by Eq. (13), can be inserted into Eq. (28) to yield $dR_S^i(T)/d\epsilon$ for $i=c$ or $i=b$. The integral in Eq. (28) can be reduced to a single quadrature, which is not expressible in terms of the usual elementary functions and was therefore evaluated numerically. We again retained only the $\vec{G}=\vec{0}$ term in the sum over reciprocal-lattice vectors which is valid for $2k_{Fc}$, $2k_{Fb}$, and κ less than half the magnitude of the smallest nonzero reciprocal-lattice vectors. Calculations were made for the values of $2k_{Fb}$ and $2k_{Fc}$ indicated above for a wide range of temperatures. The results for $dR_S^i(T)/d\epsilon$ are plotted in Fig. 3 as a function of $\log_{10}\epsilon$. For $\epsilon \gtrsim 10^{-3}$, which corresponds to $T - T_C \geq 0.3$ K in the case of Gd, it is seen that slope of $R_S^c(T)$ is negative and is an order of magnitude stronger than the slope of $R_S^b(T)$, which is initially

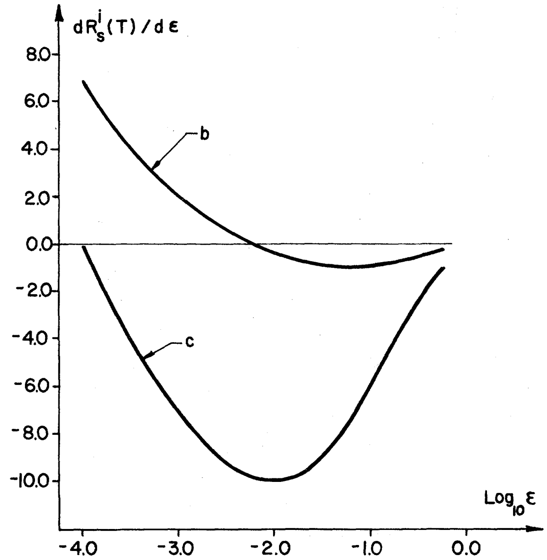

FIG. 3. Reduced temperature derivative of resistivity vs the logarithm of reduced temperature for the cylindrical-symmetry model. Curves are labeled by b and c, which refer to the direction in which the resistivity is measured.

positive but then changes sign and is very small (and would then be virtually impossible to distinguish from the phonon background). Consequently, we conclude that several features of the resistivity of type-III ferromagnets may also be accounted for by spin-fluctuation scattering, provided the Fermi-surface anisotropy is included, with the possible exception of a very small temperature region near T_C. Of course, this temperature region is a very sensitive one in complex ferromagnets, and a number of other effects may be competing with direct spin-fluctuation scattering. However, it is clear that the latter cannot be neglected.

V. SUMMARY AND CONCLUSIONS

Our objective has been the development of a simple theory which can reasonably describe, in a unified way, the three distinct types of behavior of electrical resistivity observed near the critical point of ferromagnets. Subject to reasonable simplifying approximations, it has been proved quite generally that $dR_S^i(T)/dT > 0$ and varies as the magnetic specific heat at $T = T_C^+$. This universal feature is strictly limited to $T \to T_C^+$, and as T increases above T_C, length scales other than $\xi = 1/\kappa$ become important. The most significant of these is the inverse Fermi-surface caliper, rather than the finite electron mean free path. As a consequence, large-angle scattering through $q \simeq 2k_F$ dominates both the magnitude and the temperature dependence of the resistivity in the critical range. To describe the gradual crossover from short-range dominance at T_C to "long-range" dominance at higher temperature and, in particular, the possibility of a change in sign of $dR_S^i(T)/dT$, it is therefore essential to describe correctly the spin correlations near $T_0(2k_F)$ where $T_0(2k_F)$ denotes the temperature at which $\Gamma(q = 2k_F, T)$ has its maximum as a function of T. Bearing these facts in mind, the results of Sec. IV are readily understandable. In particular, the differences between type-I and -II ferromagnets are ascribable to the role played by $T_0(2k_F)$ in the corresponding ranges of ϵ. In the case of the anisotropic Fermi surface which was used to describe type-III ferromagnets, similar roles are played by $T_0(2k_{Fc})$ and $T_0(2k_{Fb})$. It is particularly important to note that the small Fermi-surface caliper in the c direction implies that the crossover, as the temperature is lowered, from negative $dR_S^c(T)/dT$ to positive values (as required at T_C^+) occurs very close to T_C (e.g., $\epsilon < 10^{-3}$ in the model calculation of Sec. IV). This is clearly a difficult proposition to verify in detail experimentally, but it is consistent with the extremely rapid variation of $dR^c(T)/dT$ which is observed experimentally in the immediate vicinity of T_C.

We conclude that the results of our calculations of the contribution to resistivity due to spin fluctuations are consistent with all of the experimental facts indicated in Fig. 1, provided that (a) a reasonable spin correlation function is used, and (b) the effects of Fermi-surface geometry are taken into account. Of course, in a final analysis, one must not be so naive as to ignore the many other complications which exist in real systems. For example, it has been suggested that the negative slope of $R(T)$ above T_C in the case of c-axis Gd is due primarily to the anomalous thermal expansion[3] reflected in $dc(T)/dT$. There is certainly no doubt that this effect exists,[16] in addition to the usual spin-fluctuation resistivity described in Sec. IV, but we are not convinced that it plays a dominant role. A number of other effects also merit quantitative consideration. The long-range dipole-dipole forces could lead to a crossover to a regime dominated by dipolar interactions[17] in the immediate vicinity of T_C. The role of strains and sample-dependent inhomogeneities in broadening the transition should be further elucidated. Inelastic scattering and umklapp processes in systems with complex band structures should also be studied. The role of anisotropy, with respect to the crystal axes, of $\Gamma(R, T)$ may also be relevant in noncubic systems.

All of the above analysis has been limited to the paramagnetic state, $T \geq T_C$. Some remarks concerning resistivity in the ordered state below T_C are in order. There are two distinct ways in which long-range order, $\sigma(T) \propto |\epsilon|^{\beta}$, might be thought to be reflected in the resistivity. One of these was shown to be spurious by RG. A second way, of which RG were also aware, entails the long-range order appearing in the average Bloch potential for the electrons. The electron energies and velocities would thereby contribute a term to $dR(T)/dT$ which varies as $|\epsilon|^{2\beta-1}$, as pointed out by Kasuya and Kondo.[18] This effect is also spurious. The inclusion of the long-range order, or background magnetization, in the average Bloch potential is manifestly a mean-field approximation which is particularly bad near T_C. The dominant role is played by *fluctuations,* so that any electron renormalization effects must reflect the specific-heat temperature dependence for $T \to T_C^-$. This conclusion also follows from noting that $\langle \vec{S}_{\vec{R}} \cdot \vec{S}_{\vec{0}} \rangle = S(S+1)$ for $\vec{R} = \vec{0}$ in the ordered state, just as for $T > T_C$ and that the near-neighbor correlations still carry the specific-heat singularity for $T \to T_C^-$. The temperature dependence of the spin correlations for $R \gg \xi$ [which is where the $\sigma^2(T)$ term appears] is just as irrelevant for T_C^- as it is for T_C^+. The basic reason is again the fact that the electronic coherence is limited by an inherent cutoff due to the sharp Fermi surface. Consequently, only short-range correlations are reflected in the resistivity, and $dR(T)/dT$ varies as the magnetic specific heat for $T \to T_C^-$. Of course, the inclusion of long-range order in the average Bloch potential by a mean-field approximation becomes realistic somewhat below T_C, but it is then appropriate to consider also the role of electron-magnon scattering.

The methods of analysis described in this paper have also been applied to antiferromagnets. The results will be published later in a separate paper.

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