the positions of these levels. In addition to those reported here, we have performed a variety of high-field measurements on single crystals of both light and heavy rare-earth metals, and a full account of these investigations will appear in due course.

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Resistive Anomalies at the Critical Point of Isotropic Ferromagnets*

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The effect of spin fluctuations on electrical resistivity $\rho(T)$ is studied in a single-band model. It is shown that $d\rho(T)/dT$ varies as the magnetic specific heat for $T<T_c$ as well as $T>T_c$ and that both short-range and long-range correlations yield $d\rho(T)/dT>0$ for $T>T_c$.

The study of the effect of critical spin fluctuations on the electrical resistivity of metallic ferromagnets has attracted much attention. Recent reviews, to which the reader is referred for a survey of the literature, have been given by Kawatra and Budnick[1] and by Parks.[2] Theoretical discussion of resistive anomalies [i.e., singularities of $d\rho/dT=\rho'(T)$ at T_c] have been based on the s-d (or s-f) exchange model used by de Gennes and Friedel,[3] in which conduction electrons are coupled by exchange interactions to localized spins $\vec{S}_{\vec{R}}$ located at lattice sites $\vec{R}$. Assuming the electrons to be weakly and quasielastically scattered by long-lived spin fluctuations, the spin contribution to the total resistivity of an isotropic system can be written in terms of the high-temperature (spin disorder) limit ρ_0 as

$$\rho(T)/\rho_0=\sum_{\vec{R}}\Gamma(\vec{R},T)\Phi(\vec{R}), \quad (1)$$

where

$$\Gamma(\vec{R}, T) = (\langle \vec{S}_{\vec{R}} \cdot \vec{S}_{\vec{0}} \rangle - \langle \vec{S}_{\vec{R}} \rangle \cdot \langle \vec{S}_{\vec{0}} \rangle)/S(S+1) \quad (2)$$

is the spin correlation function. Its length scale is $\xi(T) = \xi_0 \epsilon^{-\nu}$, where $\epsilon = |T - T_c|/T_c$, and standard notation for critical exponents will be employed.[4] The electronic function $\Phi(\vec{R})$ is of damped oscillatory form. If the damping due to finite electron mean free path l is neglected, the explicit form in the case of a free-electron Fermi surface of radius k_F is [Eq. (9) of Fisher and Langer[5]]

$$\Phi_0(\vec{R}) = \frac{1}{4k_F{}^4 R} \frac{d^2}{dR^2}\left(\frac{\cos(2k_F R) - 1}{R}\right). \quad (3)$$

Using Eq. (3) and an Ornstein-Zernike type of approximation for $\Gamma(\vec{R}, T)$ in Eq. (1), de Gennes and Friedel[3] predicted a finite upward-pointed cusp at T_c for $\rho(T)$. This prediction disagreed with experimental results for nickel [$\rho'(T) > 0$ through T_c] and led Fisher and Langer[5] to conclude that the finite mean free path l provides a cutoff on the effectiveness of long-range correlations so that Eq. (3) might more appropriately be replaced by

$$\Phi(\vec{R}) \simeq \Phi_0(\vec{R}) e^{-R/l}. \quad (4)$$

Consequently, the short-range ($R \ll \xi$) correlations dominate resistive anomalies for sufficiently *small* $T - T_c$. This conclusion was supported by an approximate calculation, said to be valid for sufficiently large $k_F l$ and reasonable values of critical exponents, which yielded $\rho'(T) > 0$.

In this Letter, we demonstrate the following:

(1) Short-range correlations unambiguously yield $\rho'(T) > 0$, even for relatively short mean free paths,[6] but *only* if the Fermi surface is contained within the first Brillouin zone.

(2) If the current carriers are consistently described, e.g., by a single band with the Fermi surface contained within the first Brillouin zone, there exists the sum rule

$$\sum_{\vec{R}} \Phi(\vec{R}) = 0. \quad (5)$$

Use of Eq. (5) leads to the conclusion that $\rho'(T)$ varies as that magnetic specific heat *below* as well as above T_c. The $\epsilon^{2\beta-1}$ term suggested by Fisher and Langer is absent.

(3) A criterion is given for estimating the temperature range in which short-range correlations determine $\rho'(T)$. In the case of nickel, it is estimated that $\epsilon < 10^{-3}$ is required. At higher temperatures where a *long-range* correlation function is more appropriate, it is shown that $\rho'(T) > 0$ also follows subject to satisfying the "equal site" sum rule

$$\Gamma(\vec{R} = \vec{0}, T) = 1. \quad (6)$$

(4) The lattice Fourier transforms of typical *long-range* correlation functions have been studied for $T > T_c$. Provided the sum rule equation (6) is satisfied, the resulting

$$\Gamma(\vec{q}, T) = 1 + \sum_{\vec{R} \neq \vec{0}} e^{-i\vec{q}\cdot\vec{R}} \Gamma(\vec{R}, T) \quad (7)$$

has features very similar to those described in Ref. 5 for the *exact* correlation function. In particular, $d\Gamma(\vec{q}, T)/dT > 0$ for large q.

Consider first the short-range correlations *above* T_c. For small R/ξ, write Eq. (2) as[4,5,7]

$$\Gamma(\vec{R}, T) = \frac{D(\kappa R)}{(R/a)^{1+\eta}}, \quad (8)$$

where a is the lattice constant, $\kappa = 1/\xi$, and

$$D(x) = D_0 - D_1 x^{(1-\alpha)/\nu} - D_2 x^{1/\nu} + \cdots. \quad (9)$$

Use of these results and Eq. (4) in Eq. (1) leads to[5]

$$\rho'(T)/\rho_0 = A\epsilon^{-\alpha} + B + \cdots, \quad (10)$$

$$A = -D_1(\kappa_0 a)^{(1-\alpha)/\nu} \sum_{\vec{R} \neq \vec{0}} (R/a)^{\varphi} \Phi_0(\vec{R}) e^{-R/l}, \quad (11)$$

with $\varphi = -(1+\eta) + (1-\alpha)/\nu$. B is also of the form of Eq. (11), but with $D_1 \to D_2$ and $\alpha \to 0$. The sums in Eq. (11) were evaluated numerically for a fcc lattice for a wide range of values of the model parameters ($1 \leq l/a \leq 10$, $0.5 \leq k_F a \leq 10$, $0.3 \leq \varphi \leq 0.7$) with an accuracy of about 1%. D_0, D_1, $\kappa_0 a$, and critical exponents were taken from three-

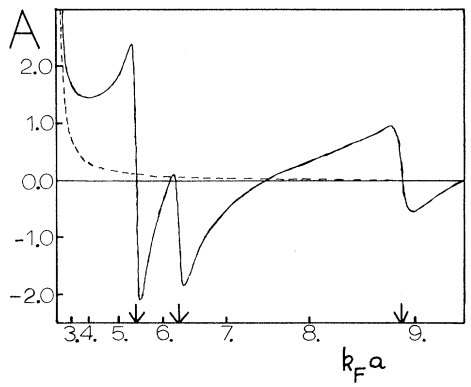

FIG. 1. The coefficient A, which determines the sign of $\rho'(T)$ in Eq. (10), as a function of $k_F a$. The corresponding integral approximation, Eq. (12), is given by the dashed line. The scale of the abscissa is linear in the variable $(k_F a)^{1/3}$ and points where $2k_F = G$ are indicated by arrows.

dimensional Ising-model calculations.[4,8,9] From this numerical study, we found $\rho'(T)$ to be quite insensitive to both φ and l/a. Thus, modest deviations from the scaling form, Eqs. (8) and (9), or errors due to improperly identifying or estimating l/a would not lead to important changes in our results. Typical results for A are plotted as a function of $k_F a$ in Fig. 1 for $\varphi = 0.5$ and $l/a = 8$. To compare with Ref. 5 we have also plotted the result obtained by replacing the sum in Eq. (11) by an integral. This approximate procedure yields the explicit form

$$A \simeq \frac{4\pi/\Omega_0}{(2k_F a)^{3+\varphi}} D_1 (\kappa_0 a)^{(1-\alpha)/\nu} \times \left[\frac{4\Gamma(\varphi+1)}{(\beta^2+1)^{(\varphi+1)/2}} \cos[(\varphi+1)\theta] + \frac{8\Gamma(\varphi-1)}{\beta^{\varphi-1}} - \frac{8\Gamma(\varphi-1)}{(\beta^2+1)^{(\varphi-1)/2}} \cos[(\varphi-1)\theta] - \frac{8\Gamma(\varphi)}{(\beta^2+1)^{\varphi/2}} \sin(\varphi\theta) \right], \quad (12)$$

where Ω_0 is the volume per ion, $\beta = (2k_F l)^{-1}$, $\theta = \tan^{-1}(2k_F l)$, and $\Gamma(x)$ is the usual Γ function.

It is evident from Fig. 1 that $\rho'(T)/\rho_0 \simeq A\epsilon^{-\alpha}$ is sensitive to the density of current carriers as specified by $k_F a$. To appreciate why, note that the point in Fig. 1 at which A first becomes negative corresponds to $2k_F = 2\pi\sqrt{3}/a = |\vec{G}_1|$, the first nonzero reciprocal-lattice vector. Similarly, the remaining sharp structure in A corresponds to $2k_F$ crossing other reciprocal-lattice vectors.

After some reflection, it is clear that considerable care is needed when specifying a physically correct set of states to describe the scattering problem. In the present case of a transition metal, we shall consider the dominant current carriers to be described by a (sp-like) dispersion law and neglect any contribution to the current from d-band conduction or interband effects.[10] In this nonfree electron description, $2k_F$ is the caliper of the s-p electron (or hole) surface. The density of these current carriers (effective valence ≤ 1) is then such that this portion of the Fermi surface is fully contained within the first Brillouin zone. Within this modified model, $\Phi_0(\vec{R})$ can be calculated just as before and Eq. (3) still applies so Fig. 1 again results. However, now the only physical range is $2k_F < G_1$. We conclude that $B > 0$ and so $\rho'(T) > 0$ for all physical values of k_F and l even though the product $k_F l$ may not be large.

There is also a more fundamental reason for rejecting the free-electron predictions for $2k_F > G_1$. A direct calculation along the lines of Eq. (1) of the resistivity in the limiting case of a weak short-range periodic potential yields

$$\rho_{per} \propto \sum_{\vec{R}} \Phi(\vec{R}). \quad (13)$$

Obviously, ρ_{per} must vanish since a periodic potential only leads to a new set of stationary states but not to resistance. However, oversimplified approximations may fail to yield zero for the sum in Eq. (13). A case in point is that of free electrons for $2k_F > G_1$. For simplicity, neglect the mean free path. Then using Eq. (3), the sum in Eq. (13) is found to be proportional to $\sum_{\vec{G}} G\theta(2k_F - G)$, where the sum is over all reciprocal-lattice vectors and does *not* vanish if $2k_F > G_1$. This unphysical feature of the free-electron approximation is responsible for the structure in Fig. 1.

The fact that scattering through reciprocal-lattice vectors plays an important role strongly suggests that a consistent treatment of lattice periodicity would restore $\rho_{per} = 0$. This is indeed the case. Recall that current decay or resistivity is due to the changes in electron *velocity* $\vec{V}(\vec{k}) = \nabla_{\vec{k}} E(\vec{k})/\hbar$ as a result of scattering. If we take account of Bloch electron velocity symmetry, it is easy to see (particularly in the reduced-zone scheme) that any electronic transitions which are induced by a periodic potential and which are permitted by energy conservation will always have exactly zero velocity transfer for arbitrary nondegenerate band structure. Thus, the sum in Eq. (13) vanishes. This conclusion also follows even if the mean free path (inelastic scattering) is included provided the dominant current carriers are well described by a single band. Thus, to the level of approximation required in the present discussion, it follows that a correct $\Phi(\vec{R})$ should satisfy Eq. (5). In simplest physical terms, Eq. (5) guarantees that imposing an additional periodic potential (such as that due to long-range order) does not lead to an additional term in the total resistivity, but only to a modification of cross sections for existing scattering processes. In practice, simple approximations to $\Phi(R)$, such as Eq. (4), will violate Eq. (5) to some degree even though $2k_F < G_1$. Fortunately, in this case, precise details of $\Phi(\vec{R})$ are not crucial when calculating real resistive processes.[11]

As an application of Eq. (5), consider the role

of the long-range order for $T > T_c$. Equation (1) can be rewritten in terms of the total spin correlation function as

$$\frac{\rho(T)}{\rho_0} = \sum_{\vec{R}} \langle \vec{S}_{\vec{R}} \cdot \vec{S}_{\vec{0}} \rangle \frac{\Phi(\vec{R})}{S(S+1)} - \frac{S^2 \sigma(T)^2}{S(S+1)} \sum_{\vec{R}} \Phi(\vec{R}), \quad (14)$$

where $\sigma(T) \propto \epsilon^{\beta}$ is the reduced magnetization. However, the last term in Eq. (14) is zero by Eq. (5), so

$$\frac{\rho(T)}{\rho_0} = 1 + \sum_{\vec{R} \neq \vec{0}} \langle \vec{S}_{\vec{R}} \cdot \vec{S}_{\vec{0}} \rangle \frac{\Phi(\vec{R})}{S(S+1)}. \quad (15)$$

We conclude that $\rho'(T)$ should vary as the observed magnetic specific heat, i.e., $\propto \epsilon^{-\alpha'}$, rather than as $\epsilon^{2\beta-1}$ as previously proposed.[5,12] This conclusion agrees with experimental data below T_c[1,2] and illustrates well the physical meaning of the sum rule.

Now consider the relative roles of short-range versus long-range correlations for $T > T_c$. A rough upper bound on the ϵ range in which short-range correlations dominate may be obtained by noting that the major contributions to sums such as Eq. (11) come from $R \lesssim 2l$. Useful approximations should maintain $\Gamma(\vec{R}, T) > 0$ in this R range so, from Eqs. (8) and (9), we require at least $D(\kappa_0 \epsilon_{SR}{}^{\nu} 2l) \geq 0$ for $\epsilon \leq \epsilon_{SR}$. If we use available data for three-dimensional Ising models[4,8] to estimate coefficients, $\epsilon_{SR} \simeq 1.8 \times 10^{-3}$. In the case of Ni, this corresponds to $\Delta T \lesssim 1.1$°K. Since the resistive anomaly in Ni is present over a much wider range of ΔT, it is essential to reconsider the role of long-range correlations. To do so, we used the generalized Ornstein-Zernike (GOZ) approximations of Ferer, Moore, and Wortis,[8,13]

$$\Gamma_{GOZ}(\vec{R}, T) = C(\kappa a)^{\eta}(a/R) e^{-\kappa R}, \quad (16)$$

which is applicable for $\kappa a > 0.1$, i.e., $\epsilon > \epsilon_{LR} \simeq 7.5 \times 10^{-3}$ or $\Delta T \gtrsim 4.7$°K in the case of Ni. We have used Eqs. (4) and (16) in Eq. (1) and evaluated the sums numerically for a fcc lattice. In Fig. 2, we have plotted a typical set of results for $\rho_{GOZ}(T)/\rho_0$ as a function of κa. It is seen that $\rho'(T) > 0$ in the entire temperature range, $\kappa a > 0.1$, of validity of GOZ. We have also carried out lattice sums using the well-known Ornstein-Zernike (OZ) approximation [i.e., $\eta = 0$ in Eq. (16)] for $R \geq a$ and the sum rule (6) for $R = 0$. In this approximation, we also found $\rho_{OZ}'(T) > 0$. This is in striking contradiction to the common (and incorrect) belief that long-range correlations inevitably result in $\rho'(T) < 0$.

To appreciate what is involved, consider the

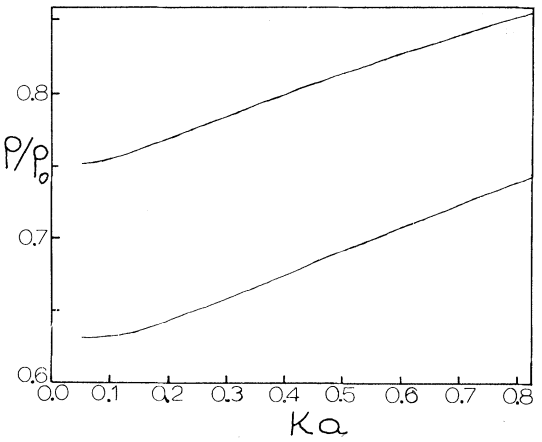

FIG. 2. Normalized resistivity in the GOZ approximation (see text) as a function of κa for $l/a = 8$. The upper (lower) curve corresponds to an effective carrier valence of 1.0 (0.5).

lattice Fourier transform, Eq. (7), in the simple OZ approximation. To evaluate $\Gamma(\vec{q}, T)$ for small q and κ, the sum in Eq. (7) is often replaced by a Fourier integral and the usual $\Gamma_{OZ}(\vec{q}, T) \simeq (4\pi C a/\Omega_0)/(\kappa^2 + q^2)$ follows. However, this misrepresents the T dependence of $d\Gamma(\vec{q}, T)/dT$, and a more careful asymptotic expansion is required. By converting Eq. (7) into a sum over reciprocal-lattice vectors, the dominant terms can be isolated and yield

$$\Gamma_{OZ}(\vec{q}, T) = 1 + Ca\left[\frac{4\pi/\Omega_0}{\kappa^2 + q^2} + \kappa - b + O(q^2, \kappa^2)\right], \quad (17)$$

where b is a lattice-dependent constant. It is clear from Eq. (17) that for fixed q, $\Gamma_{OZ}(\vec{q}, T)$ has a maximum as a function of T at $T = T_0(q) > T_c$ and that $d\Gamma_{OZ}(\vec{q}, T)/dT \gtrless 0$ for $T \gtrless T_0(q)$.[14] In fact, $\Gamma_{OZ}(\vec{q}, T)$ qualitatively resembles the *exact* correlation function sketched in Fig. 1 of Ref. 5. Recalling Fisher and Langer's argument that $\rho'(T)$ and $d\Gamma(\vec{q}, T)/dT$ for large q are of the same sign, it becomes clear why OZ and GOZ long-range correlation functions and the Fisher-Langer short-range form all lead to $\rho'(T) > 0$.

In summary, the above conclusions provide a consistent description of isotropic nickel-like ferromagnets. Applications to more complex systems will be described elsewhere.

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[10]This is the simplest view which can be reasonably reconciled with transition-metal band structure.

[11]We have recalculated the lattice sums for A using approximations to $\Phi(\vec{R})$, other than $e^{-R/l}\Phi_0(\vec{R})$, which satisfy the sum rule Eq. (5) to high accuracy. The results for A were virtually unchanged from those in Fig. 1 for $2k_F < G_1$.

[12]More generally, $\Phi(\vec{R})$ is a tensor, albeit diagonal in isotropic cases. It is only $\Phi^{zz}(\vec{R})$ which enters the second term in Eq. (14), but the sum vanishes at any rate.

[13]Of course, the $R = 0$ point is given by Eq. (6) and the proposed form for $\Gamma(\vec{R}, T)$ applies only for $R \geq a$.

[14]The structure implied by the change in sign of $d\Gamma(\vec{q}, T)/dT$ is fairly general and necessary to satisfy the equal-site sum rule in the form $d\Gamma(\vec{R}=\vec{0}, T)/dT = 0$.

Consistent Test of the Strutinsky-Nilsson Method*

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The Strutinsky method for extracting the shell corrections from Nilsson single-particle energies is tested consistently within the constrained Hartree-Fock (CHF) framework. It is shown that a Nilsson potential, fitted to the CHF single-particle energies at one deformation, reproduces the CHF level ordering at other deformation surprisingly well. The shell corrections obtained from the Nilsson single-particle energies via the Strutinsky method are shown, however, to be unreliable by 30% on the average.

The Strutinsky-Nilsson[1] (SN) procedure for obtaining energy-deformation surfaces for nuclei consists of the following steps: (a) Nature supplies single-particle energies $\mathcal{E}_n$ at the ground-state deformation and the total binding energy. (b) The parameters of the Nilsson potential are adjusted to optimally reproduce these $\mathcal{E}_n$, and the potential thus obtained generates single-particle energies $\mathcal{E}_n(Q)$ as a function of deformation. (c) The smoothly varying part of the sum of the $\mathcal{E}_n(Q)$ up to the Fermi level, as a function of deformation, is extracted using the Strutinsky averaging procedure, and the remainder is interpreted as the shell correction. (d) The smoothly varying part of the energy is obtained from a liquid-drop model (LDM) which is fit to the total binding energies of all nuclei. (e) The energy deformation surface, obtained by adding the shell corrections to the LDM energy as a function of deformation, is compared with the "experimental" energy deformation surface by considering fission half-lives, etc.

In the work of Bassichis *et al.*[2] it was pointed out that there are three wave functions or density matrices which must be considered in order to interpret the SN method within the CHF framework. Let ρ be the CHF density matrix leading to energy E at some quadrupole moment Q_0. Let $\bar{\rho}$ be some smoothly varying (with Q) density matrix which generates a smoothly varying sin-