spondingly larger. The analysis was done with $\nu = 0.638$ and $\nu = 0.625$. Results are shown in Table II. OZ values for the two moments shown are 7.425 and 10.929.

If $\nu = 0.638$, then these results are consistent with universality. If $\nu = 0.625$ ($\eta = 0$), then our extrapolations are in suggestive agreement with OZ. The close connection between ν and the moment-ratio extrapolants precludes resolution of this ambiguity.

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[1]M. E. Fisher, Rept. Progr. Phys. 30, 615 (1967); L. P. Kadanoff *et al.*, Rev. Mod. Phys. 39, 395 (1967).

[2]P. Heller, Rept. Progr. Phys. 30, 731 (1967).

[3]David Jasnow and Michael Wortis, Phys. Rev. 176, 739 (1968); R. B. Griffiths, Phys. Rev. Letters 24, 1479 (1970).

[4]For example, if universality fails, then it is unlikely that there exists a unique critical operator algebra for each dimensionality and symmetry. See L. P. Kadanoff, Phys. Rev. Letters 23, 1430 (1969).

[5]C. Domb, Advan. Phys. 9, 149 (1960); C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) A240, 214 (1957).

[6]Spin dependence of the Ising and Heisenberg models was first studied by C. Domb and M. F. Sykes, Phys. Rev. 128, 168 (1962). Heisenberg-model work was also done by ($S = \frac{1}{2}$) G. A. Baker *et al.*, *ibid.* 164, 800 (1967), and ($S = \infty$) H. E. Stanley, *ibid.* 158, 537 (1967), and has been recently reanalyzed by R. G. Bowers and M. E. Woolf, *ibid.* 177, 917 (1969).

[7]More recent work on the spin-S Ising model using 12-term high-temperature series suggests the presence of confluent singularities in the susceptibility and other moments: D. M. Saul, David Jasnow, and Michael Wortis (unpublished). The apparent spin dependence of γ found in an earlier publication (Jasnow and Wortis, Ref. 3) can be explained in this way while maintaining $\gamma = 1.25$ for all S. The status of ν is less clear. Present data admit a range of values $0.62 < \nu < 0.64$ for $S > \frac{1}{2}$.

[8]P. G. Watson, J. Phys. C 2, 1883 (1969); D. S. Gaunt and C. Domb, *ibid.* 3, 1442 (1970).

[9]L. P. Kadanoff, Physics 2, 263 (1966); M. E. Fisher and R. J. Burford, Phys. Rev. 156, 583 (1967).

[10]M. Ferer, M. A. Moore, and Michael Wortis, Phys. Rev. Letters 22, 1382 (1969). There is evidence that (1) fails in the strong scaling limit $\kappa r \to 0$; however, the divergent moments of $\Gamma(\vec{r}, T)$ do not probe this region. Our discussion is therefore limited to the "weak scaling" universality of $D(x)$. See also G. Stell, *ibid.* 24, 1343 (1970).

[11]It is expected, for example, that nearby sites contribute energy-density-like terms $(1 + C\epsilon^{1-\alpha} + \cdots)$. For spins other than $S = \frac{1}{2}$ there appear to be further divergent terms, more singular than $\kappa^{-n-2+\eta}$.

[12]A proof that the correlations have OZ form $T > T_c$, $r \to \infty$ is given by W. J. Camp, thesis (Cornell University, 1970) (unpublished), and M. E. Fisher and W. J. Camp, Phys. Rev. Letters 26, 73 (1971).

[13]M. A. Moore, David Jasnow, and Michael Wortis, Phys. Rev. Letters 22, 940 (1969).

[14]M. F. Sykes, J. L. Martin, and D. L. Hunter, Proc. Phys. Soc. (London) 91, 671 (1967).

[15]Note that convergence is best when $y \gg x$. For this reason we have avoided ratios (4) with weakly singular demoninators.

[16]D. R. Hartree, *Numerical Analysis* (Oxford U. P., London, 1952).

[17]A. A. Migdal, Zh. Eksperim. i Teor. Fiz. 59, 1015 (1970) [Sov. Phys. JETP (to be published)].

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Effect of Band Structure on Spin Fluctuations in Nearly Antiferromagnetic Metals

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A model band structure due to Rice which exhibits a "cusp" Kohn singularity has been used to evaluate the dynamic susceptibility of nearly itinerant antiferromagnets. The spin-fluctuation dispersion relation is derived for such systems, and it is shown that the contribution of the spin fluctuations to the electronic specific heat contains anomalous terms in contrast with the calculations of Moriya.

I. INTRODUCTION

The behavior of spin fluctuations in nearly ferromagnetic metals and alloys has been the subject of many recent research papers.[1] However, spin fluctuations in nearly antiferromagnetic metals and alloys have received little attention. There are two reasons for this situation: (i) The only itinerant antiferromagnets that have been thoroughly investigated experimentally are pure Cr and its alloys. (ii) The band structure of Cr is essential for an understanding of the nature of the antiferromagnetic ground state which is a longitudinal-linear-spin-density-wave state (LSDW) at low temperatures.[2] Since the band structure is complicated, it has been replaced by a variety of simple models for calculation purposes. For example, Sinha, Liu, Muhlestein, and Wakabayashi[3] have used a one-band parabolic model to calculate the dynamic susceptibility of Cr and obtained the following form for dynamic susceptibility:

$$\chi(\vec{q},\ \omega)=\chi^{(0)}(\vec{q},\ \omega)[1-V\chi^{(0)}(\vec{q},\ \omega)]^{-1}\ , \qquad (1)$$

in the random-phase approximation (RPA). V is the strength of the exchange interaction between conduction electrons. The tendency to antiferromagnetism results from the nesting of the Fermi surface into itself with wave vector $Q=2k_F$, where k_F is the Fermi momentum. In the limit of low frequency and small $|\vec{q}-\vec{Q}|$, the dynamic susceptibility $\chi^{(0)}(\vec{q},\ \omega)$ for the noninteracting system is given by

$$\mathrm{Re}\chi^{(0)}(\vec{q},\ \omega)=\chi_T^{(0)}(2k_F,\ 0)-a^2(\omega^2+V_F^2\,|\vec{q}-\vec{Q}\,|^2)\ ,$$
$$\mathrm{Im}\chi^{(0)}(\vec{q},\ \omega)=b\,\omega\ , \qquad (2)$$

where a and b are constants which depend on the temperature T assumed greater than the Néel temperature. Sinha *et al.*[3] were able to fit $\chi(\vec{q},\ \omega)$ given by (1) and (2) to magnetic neutron scattering data for Cr at temperatures greater than the Néel temperature T_N. The peaks in $\chi(\vec{q},\ \omega)$ as a function of $\vec{q}$ near $\vec{Q}$ indicate the presence of large-amplitude spin fluctuations in this temperature region. A similar one-band model is under investigation by Héritier and Lederer[4] to explain the giant electronic specific heat of $B_2Cr_xV_{1-x}$ in terms of spin fluctuations in nearly antiferromagnetic alloys.

II. TWO-BAND MODELS

Other models have attempted to take into account the detailed band structure of Cr. The LSDW in chromium is formed by the nesting of two similar portions of the Fermi surface separated by a vector $\vec{Q}$ which is close to half a reciprocal-lattice vector. One of these surfaces is a hole octahedron centered at the point H in the Brillouin zone of bcc Cr, and the other is the flat part of the "electron jack" centered at Γ.[5] In consequence, the one-band model must be replaced by a two-band model which attempts to simulate the real Fermi surface of Cr.

The first such model is due to Fedders and Martin,[6] who proposed that the true Fermi surface of Cr be replaced by two equal spheres (one-hole sphere and one-electron sphere) separated by a vector $\vec{Q}_0=\frac{1}{2}K_0$, where K_0 is a reciprocal-lattice vector. The LSDW ground state is stabilized by the formation of bound interband particle-hole pairs. In the paramagnetic state the intraband susceptibility defined in (1) must now be replaced for $\vec{q}$ near $\vec{Q}_0$ by an interband susceptibility given by

$$\chi_{12}(\vec{q},\ \omega)=\chi_{12}^{(0)}(\vec{q},\ \omega)[1-\tilde{V}\chi_{12}^{(0)}(\vec{q},\ \omega)]^{-1}\ , \qquad (3)$$

where $\tilde{V}$ is an interband exchange interaction and $\chi_{12}^{(0)}(\vec{q},\ \omega)$ is defined by

$$\chi_{12}^{(0)}(\vec{q},\ \omega)=\sum_k \frac{f(\epsilon_{k+q}^{(2)})-f(\epsilon_k^{(1)})}{\omega-\epsilon_{k+q}^{(2)}+\epsilon_k^{(1)}+i\delta}\ , \qquad (4)$$

where $f(\epsilon)$ is the Fermi distribution function, $\epsilon_k^{(2)}$ is the dispersion relation of the electron band corresponding to the "hole" surface, and $\epsilon_k^{(1)}$ is that corresponding to the electron surface. $\chi_{12}^{(0)}$ in (4) has been evaluated by Rice *et al.*[7] for zero frequency and momenta $\vec{q}$ close to $\vec{Q}_0$ using the Fedders-Martin model and is given by

$$\chi_{12}^{(0)}(\vec{q},\ 0)=\ln(2k_F\,/\,|\vec{q}-\vec{Q}_0|)\ , \qquad (5)$$

at zero temperature. The expression for $\chi_{12}(\vec{q},\ 0)$ obtained from (3) and (5) shows that a stable spin-density-wave ground state exists for all nonzero values of the interband coupling constant $\tilde{V}$. This is clearly incorrect. Apart from this deficiency, the Fedders-Martin model gives a good qualitative picture of the behavior of a two-band itinerant antiferromagnet.[2]

Recently, Moriya[8] has proposed that spin fluctuations in nearly antiferromagnetic metals do not contribute anomalous terms to the electronic specific heat $C_v(T)$ contrary to the case of nearly ferromagnetic metals.[1] His work is based on a one-band model where the dynamic susceptibility is given in the RPA by Eq. (1). On general grounds he shows that the zero-temperature dynamic susceptibility $\chi^{(0)}(\vec{q},\ \omega)$ in the absence of interactions is given in the limit of low frequency and small momenta $\vec{q}-\vec{Q}$ by

$$\mathrm{Re}\chi_0(\vec{q},\ \omega)=\chi_0(\vec{Q})[1-a(\vec{Q})(\vec{q}-\vec{Q})^2 - b(\vec{Q},\ \vec{q}-\vec{Q})\omega^2+\cdots]\ ,$$
$$\mathrm{Im}\chi_0(\vec{q},\ \omega)=\chi_0(\vec{Q})[c(\vec{Q},\ \vec{q}-\vec{Q})\omega + d(\vec{Q},\ \vec{q}-\vec{Q})\omega^3+\cdots]\ . \qquad (6)$$

The absence of anomalous effects in $C_v(T)$ is ascribed to the fact that $c(\vec{Q},\ \vec{q}-\vec{Q})$ stays finite as $\vec{q}\to\vec{Q}$. However, the validity of the expansion in (6) depends critically on the band structure of the metal in question.

Rice[1,9] has proposed that the band structure of Cr group metals exhibits a logarithmic Kohn anomaly which results in a "cusp" singularity in $\chi_{12}^{(0)}(\vec{q},\ 0)$ when $\vec{q}=\vec{Q}$. He was able to explain the pressure dependence of the Néel temperature using such a "cusp" model. In Sec. III, the dynamic susceptibility for a two-band model with a "cusp" Kohn singularity is derived. It is shown that Moriya's expansion (6) is not valid for this model and that, in consequence, the electronic specific heat may exhibit anomalous terms.

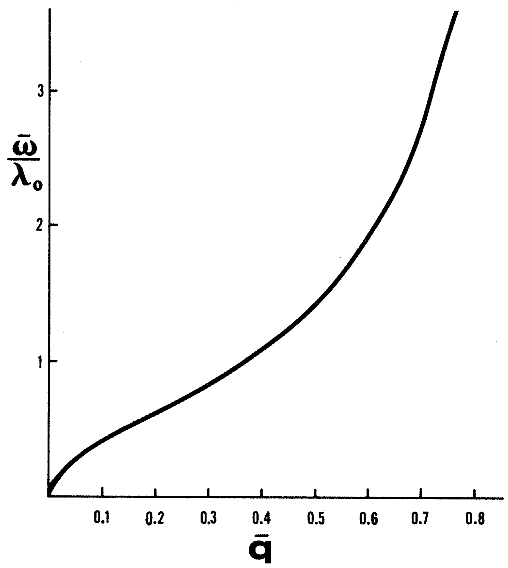

FIG. 1. Dispersion relation of the spin fluctuations in the limit $|q'| \gg \omega$.

III. SPIN FLUCTUATIONS FOR "CUSP"-TYPE KOHN SINGULARITY

The interband susceptibility $\chi_{12}^{(0)}(\vec{q}, \omega)$ defined in (4) can be written as follows for a general band structure[2,9]:

$$\chi_{12}^{(0)}(\vec{q}, \omega) = \int d\xi \int d\eta \, N_q(\xi, \eta) \, \frac{f(\eta+\xi) - f(\eta-\xi)}{\omega - 2\xi + i\delta} , \tag{7}$$

where $N_q(\xi, \eta)$ is the double density of states given by

$$N_q(\xi, \eta) = \sum_k \delta[\xi - \tfrac{1}{2}(\epsilon_{k+q}^{(2)} - \epsilon_k^{(1)})]\delta[\eta - \tfrac{1}{2}(\epsilon_{k+q}^{(2)} + \epsilon_k^{(1)})] . \tag{8}$$

Rice[9] has derived $N_q(\xi, \eta)$ for a two-band model with the following band structure:

$$\epsilon_{k+Q}^{(2)} = V_F k_z + \frac{k_x^2}{2m_x} - \frac{k_y^2}{2m_y} ,$$
$$\epsilon_k^{(1)} = - V_F k_z + \frac{k_x^2}{2m_x} - \frac{k_y^2}{2m_y} . \tag{9}$$

The resulting expression for $N_q(\xi, \eta)$ exhibits a logarithmic Kohn anomaly:

$$N_q(\xi, \eta) = \nu_0 \ln\left(\frac{\eta_0}{\eta - \frac{1}{2}q'}\right), \quad \nu_0 = \frac{m_x^{1/2} m_y^{1/2}}{4\pi^3} \tag{10}$$

where $q' = V_F(\vec{q} - \vec{Q}_0)_z$ and η_0 is the energy cutoff in the $k_x - k_y$ plane. From (7) and (10) the imaginary part of $\chi_{12}^{(0)}(\vec{q}, \omega)$ is given by

$$\mathrm{Im}\chi_{12}^{(0)}(\vec{q}, \omega) = \frac{\pi\nu_0}{2}\left(\omega(\ln\eta_0 - 1) + \frac{q'}{2}\ln\left|\frac{\omega - q'}{\omega + q'}\right| - \frac{\omega}{2}\ln\left|\frac{q'^2 - \omega^2}{4}\right|\right) . \tag{11}$$

It follows directly from Rice's work[9] that $\mathrm{Re}\chi_{12}^{(0)}(\vec{q}, \omega)$ in the low-frequency small q' limit is written as

$$\mathrm{Re}\chi_{12}^{(0)}(\vec{q}, \omega) = \nu_0(A_0 - \tfrac{1}{2}\pi^2|q'|) + O(\omega^2, q'^2) , \tag{12}$$

where A_0 is given by

$$A_0 = 2\eta_0[2 + \ln(\omega_0/\eta_0)] . \tag{13}$$

ω_0 is the energy cutoff in the k_z direction. Equation (12) shows that $\chi_{12}^{(0)}(\vec{q}, 0)$ exhibits a "cusp" at $q' = 0$ or $q = Q$. The limiting forms of $\mathrm{Im}\chi_{12}^{(0)}(\vec{q}, \omega)$ are given by

$$\mathrm{Im}\chi_{12}^{(0)}(\vec{q}, \omega) \approx \begin{cases} \frac{1}{2}(\nu_0\pi)\omega[\ln(2\eta_0/\omega) - 1] , & \omega \gg |q'| \quad (14a) \\ \frac{1}{2}(\nu_0\pi)\omega\ln(\eta_0/0.27|q'|) , & \omega \ll |q'| . \quad (14b) \end{cases}$$

It is important to note that $\chi_{12}^{(0)}$ as given in (12) and (14) for a "cusp" Kohn singularity cannot be expanded in the form (6) due to Moriya.[8] This has important consequences on the specific heat $C_v(T)$ (see below).

The spin-fluctuation spectrum $\omega_{q'}$ is given by the poles of the full interband susceptibility $\chi_{12}(\vec{q}, \omega)$ defined in (3):

$$1 \approx \tilde{V}\chi_{12}^{(0)}(\vec{q}, \omega_{q'}) . \tag{15}$$

Equations (12), (14), and (15) give the following expression for $\omega_{q'}$ in the limit $|q'| \gg \omega$:

$$\omega_{q'} = \pm \frac{2i}{\pi\nu_0\tilde{V}}(1 - \nu_0 A_0\tilde{V})\ln\left(\frac{\eta_0}{0.27|q'|}\right) . \tag{16}$$

In nondimensional units $\omega_{q'}$ becomes (see Fig. 1)

$$\bar{\omega}_q = \pm i\lambda_0 \ln(1/|\bar{q}'|) , \tag{17}$$

where

$$\bar{\omega} = 0.27\omega/\eta_0, \quad \bar{q}' = 0.27q'/\eta_0 , \tag{18}$$

and

$$\lambda_0 = 2.2[2 + \ln(\omega_0/\eta_0)]\kappa_0^2/\pi(1 - \kappa_0^2) . \tag{19}$$

κ_0^2 is the inverse of the enhancement factor given by

$$\kappa_0^2 = 1 - \nu_0 A_0 \tilde{V} . \tag{20}$$

Clearly, $\kappa_0^2 < 0$ for an itinerant antiferromagnetic, and $\kappa_0^2 \gtrsim 0$ for a nearly antiferromagnetic itinerant metal. The imaginary part of $\chi_{12}(\vec{q}, \omega)$ corresponding to (17) is given from (12), (14), and (15) by

$$\mathrm{Im}\chi_{12}(\bar{\vec{q}}, \bar{\omega}) = \frac{\pi\nu_0\eta_0}{0.27}\,\frac{\bar{\omega}\ln(1/|\bar{q}'|)}{(\lambda_0 + \frac{1}{2}\pi|\bar{q}'|)^2 + \bar{\omega}^2\ln(1/|\bar{q}'|)} . \tag{21}$$

$\mathrm{Im}\chi_{12}(\bar{q}, \bar{\omega})$ has a pronounced peak as a function of $\bar{\omega}$ when $\kappa_0^2 \gtrsim 1$ which should be observable by neutron scattering.

In the limit $|q'| \ll \omega$, the spin-fluctuation spectrum is obtained from (12), (14a), and (15). The dispersion relation is then given by

$$\omega_{q'}\left[\ln\left(\frac{2\eta_0}{\omega_{q'}}\right) - 1\right] = \pm i\left(\frac{2\kappa_0^2}{\tilde{V}\nu_0\pi} + \tfrac{1}{2}\pi|q'|\right) . \tag{22}$$

Expansion in powers of q' gives

$$\omega_{q'} = \pm i(\alpha + \beta|q'|) , \tag{23}$$

where

$$\alpha = \frac{2\kappa_0^2}{\tilde{V}\nu_0\pi[\ln(2\eta_0/\Omega_0) - 1]} , \quad \beta = \frac{\pi}{2[\ln(2\eta_0/\Omega_0) - 1]} ; \tag{24}$$

Ω_0 is the frequency of the zero-momentum spin fluctuation. Equation (23) shows that the spin fluctuations in nearly antiferromagnetic metals with a "cusp" Kohn singularity in the band structure have a phononlike dispersion relation similar to that of nearly ferromagnetic metals.[1] It is important to note that $\Omega_0 \to 0$ as $\kappa_0^2 \to 0$ [see Eq. (22)].

Recently, Jérome[10] extended the work of Moriya[8] to a two-band model with a spherical electron Fermi surface and an ellipsoidal hole Fermi surface. Moriya's expansion of $\chi(\vec{q}, \omega)$ in (6) is valid for Jérome's band structure and gives the following dispersion relation for the spin fluctuations:

$$\omega_{q'}^{J} = \pm i(\alpha' + \beta'|q'|^2) . \tag{25}$$

The different character of the dispersion relations given by Eqs. (23) and (25), respectively, indicates the importance of band-structure details in the calculation of the dynamic susceptibility. Moriya[8] has shown that the dominant contribution of the spin fluctuations to the free energy is given by

$$\Delta F = \frac{3}{2\pi} \sum_q \int_0^\infty d\omega \coth\left(\frac{\omega}{2kT}\right) \times \tan^{-1}\left(\frac{\tilde{V}\,\mathrm{Im}\chi_{12}^{(0)}(\vec{q}, \omega)}{1 - \tilde{V}\,\mathrm{Re}\chi_{12}^{(0)}(\vec{q}, \omega)}\right) . \tag{26}$$

The most important contribution to ΔF at low temperatures comes from the form of $\mathrm{Im}\chi_{12}^{(0)}(\vec{q}, \omega)$ in the limit $\omega \gg |q'|$. This contribution is obtained from (12), (14a), and (26):

$$\Delta F = \frac{3\tilde{V}}{2\pi} \int_0^{q'_c} dq' \int_0^{\omega_c} d\omega \coth\left(\frac{\omega}{2kT}\right) \times \left(\frac{\omega[\ln(2\eta_0/\omega) - 1]}{\kappa_0^2 + \frac{1}{4}\tilde{V}\pi^2\nu_0 q'}\right) . \tag{27}$$

Integration of the right-hand side of (27) and differentiation with respect to T gives the following anomalous terms in the electronic specific heat (see also Ref. 4):

$$C_v^{\mathrm{SF}}(T) \approx -AkT\ln\kappa_0(1 - B\ln T), \tag{28}$$

where A and B are constants. In particular, $C_v^{\mathrm{SF}}(T)$ becomes infinite as κ_0 goes to zero. This is identical for nearly ferromagnetic metals and is due to the choice of band structure.

IV. CONCLUSION

It has been shown in Sec. II that band-structure effects are critical in determining the excitation spectrum of spin fluctuations in neraly antiferromagnetic metals. In particular, the choice of a band structure with a "cusp" Kohn singularity has the following advantages over band structures of the Fedders-Martin type:

(i) A critical criterion for stability of an antiferromagnetic state at $T = 0$ is obtained using the "cusp" model[9] ($1 = \tilde{V}\nu_0 A_0$) in contrast to the Fedders-Martin model. Critical criteria also are obtained by using the band-structure models of Liu[11] and Jerome.[10]

(ii) The model exhibits large-amplitude spin fluctuations at zero temperature when $1 \gtrsim \tilde{V}\nu_0 A_0$. The frequency of such spin fluctuations vanishes when the critical criterion (i) is satisfied.

(iii) Anomalous behavior in the electron specific heat analogous to that of a nearly ferromagnetic metal is a consequence of the "cusp" model. This behavior is absent when a less-singular band structure is used.[8,10]

The "cusp" model may also be used for the calculation of the dispersion relation of spin waves in Cr. The Fedders-Martin model gives a spin-wave dispersion relation which is independent of the exchange coupling $\tilde{V}$ at zero temperature.[2] A calculation using the "cusp" model should give a spin-wave dispersion relation of the form

$$\omega_{q'}^{sw} = D|q'| , \tag{29}$$

when the stiffness coefficient D vanishes at the critical point, i.e.,

$$\lim D = 0 \quad \text{as} \quad \kappa_0 A_0 \tilde{V} \to 1^+ . \tag{30}$$

Work is in progress to determine D explicitly in terms of the energy gap of the antiferromagnetic state.

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[1]N. Berk and J. R. Schrieffer, Phys. Rev. Letters 17, 433 (1966); S. Doniach and S. Englesberg, *ibid.* 17, 750 (1966).

[2]For a review, see T. M. Rice, Lecture Notes, Canadian Association of Physicists Summer School on Metal Physics, Banff, Alberta, 1969 (unpublished).

[3]S. K. Sinha, S. H. Liu, D. Muhlestein, and N. Wakabayashi, Phys. Rev. Letters 23, 311 (1969).

[4]M. Héritier and P. Lederer, J. Phys. (Paris) (to be published).

[5]W. M. Lomer, Proc. Phys. Soc. (London) 80, 489 (1962).

[6]P. A. Fedders and P. C. Martin, Phys. Rev. 143, 245 (1965).

[7]T. M. Rice, A. S. Barber, Jr., B. I. Halperin, and D. B. McWhan, J. Appl. Phys. 40, 1337 (1969).

[8]T. Moriya, Phys. Rev. Letters 24, 1433 (1970).

[9]T. M. Rice, Phys. Rev. B 2, 3619 (1970).

[10]D. Jérome, Solid State Commun. 8, 1793 (1970).

[11]S. H. Liu, Phys. Letters 27A, 493 (1968).