a theory does not exist for the type of system studied here. However, the apparently simple relation between the coefficient of the T^2 low-temperature dependence of ρ_m, the total spin-disorder scattering $\Delta\rho_m$ and the iron concentration, together with the consistency of the interpretation of our data in terms of electron-magnon scattering with an effective concentration dependent s-d exchange integral, suggest that such a theory should be obtainable from a complete treatment of the s-d scattering mechanisms in terms of the dynamic susceptibility $\chi(\vec{q}, \omega)$ for *Pd*Fe. A recent paper[24] has considered in some detail the properties of this function and shows that the spin-wave excitations are damped. This should have an important effect on the electron-magnon scattering.

Note added in proof. All of the experiments reported in this paper were performed in zero applied magnetic field. The effect of the demagnetizing field on the resistance is not considered in this study.

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Band-Structure Effects in Itinerant Antiferromagnetism

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The effect of imperfect "nesting" of the band structure on itinerant antiferromagnetism is considered. A model band structure with spherical electron and hole pockets of unequal radii and a "nonmagnetic" reservoir is examined. A first-order commensurate-incommensurate transition is found, but the paramagnetic transition remains second order. The influence of generalized Kohn anomalies on the transition is investigated, and it is found that though they lead to anomalous behavior in the limit of vanishing antiferromagnetism, there is no change in the order of the transition.

I. INTRODUCTION

In recent years, the antiferromagnetism of Cr and its alloys has been studied extensively. It has been well established that the antiferromagnetism in Cr and its alloys is itinerant in nature and is an example of an Overhauser spin density wave arising from correlations between the conduction electrons.[1] The importance of the peculiar nature

of the Cr Fermi surface, in which there are large electron and hole pockets similar in size and shape, was first emphasized by Lomer.[2] Much of the subsequent theoretical analysis of Cr has employed simplified models of the band structure in which it is assumed that the "nesting" between the electron and hole pockets is perfect.[3]

In this paper we will be concerned about the effects of imperfect nesting on itinerant antiferromagnetism. We will study in a Hartree-Fock approximation a number of simple model band structures, in order to gain insight into the influence of various aspects of the band structure on such properties as the variation of the Néel temperature T_N with changes in the band structure due to pressure or alloying, the variation of Q-vector with temperature and band-structure changes, etc. One question which we had hoped to investigate was the question of first- versus second-order transitions at T_N. However, all of the models which we have investigated have a second-order phase transition between the paramagnetic and antiferromagnetic phases, whereas the observed transition in Cr is first order, though weakly so.

We will restrict ourselves in this paper to the weak-coupling limit and work within a simple Hartree-Fock approximation. We will make a further approximation of keeping only the dominant term in the Hamiltonian which describes the Coulomb attraction between the electrons and holes. We ignore the intraband exchange interactions and the coupling between the "magnetic" portions of the Fermi surface and the "nonmagnetic" portions, i.e., those parts which are not substantially affected by the transition. For the case of the Cr Fermi surface, this corresponds to the retention of the interaction between the hole octahedron centered at H and the body of the electron jack centered at Γ and the omission of the coupling to the balls on the electron jack and the hole ellipsoids at N. We make the additional approximation of replacing the screened Coulomb interaction by a constant, and of ignoring the change in screening associated with the loss of carriers in the antiferromagnetic phase. It is possible that by going beyond these approximations qualitative changes can occur in the behavior of the system, such as a change from a second-order transition to a first-order one. In the few cases where this has been investigated, however, no qualitative changes were found.

In Sec. II, we will examine the itinerant antiferromagnetic transition for a model band structure with imperfect nesting. The model band structure has one electron pocket, one hole pocket, and a nonmagnetic background. The electron and hole pockets are taken as spherical in shape. If the radii of the two pockets are equal, then the model has perfect nesting but we will allow the radii to differ, leading to imperfect nesting. The model has certain mathematical similarities to the effect of Pauli paramagnetism on the BCS theory of superconductivity which has been studied by a number of authors.[4-7] The existence of the nonmagnetic portion of the Fermi surface (not involved in the antiferromagnetic transition) gives us an additional variable, and there is complete mathematical equivalence to superconductivity only in one limit. We find that in this model the paramagnetic to antiferromagnetic transition is always second order. There are, however, first-order transitions between antiferromagnetic states with different periods similar to the commensurate-noncommensurate transition observed in some Cr alloys.[8] Such transitions were predicted on general grounds by Herring[9] and discussed in detail for a one-dimensional model by Falicov and Penn.[10] The suggestion that the changes in the antiferromagnetism in certain Cr alloys were due to the relative variation of the electron and hole portions of the Fermi surface with the changing electron to atom ratio was first made by Muheim and Muller.[11]

In Secs. III and IV, we investigate the possible influence of generalized Kohn anomalies[12,13] on the transition. In Sec. III, we discuss a model band structure in which the one-electron-band susceptibility has its maximum at a "cusp"-type anomaly. It has been shown that such cusp-type Kohn anomalies must occur in the Cr-group metals and that in the particular case of W a maximum in the one-electron susceptibility occurs at a cusp-type anomaly.[14] This feature of the band structure leads to an anomalous variation of T_N with external parameters, such as pressure in the neighborhood of the point where the Néel temperature goes to zero. We find that transition remains second order, however, at least in the weak-coupling limit.

In Sec. IV, we turn our attention to higher-order cusp-type Kohn anomalies, which may occur at points of high symmetry. We also discuss, in some detail, the case of a cylindrical Kohn anomaly.[13] While an anomaly of this kind cannot really occur in nature, it may nevertheless be a useful approximation to represent a complicated series of anomalies by such a cylindrical anomaly over a limited region of wave vector.

Finally, in Sec. V, we state the conclusions and make some remarks concerning the question of first- versus second-order transitions in itinerant antiferromagnetism.

II. UNEQUAL SPHERE MODEL

In this section, we shall consider a model Fermi surface with two spherical pockets, one of electrons and the other of holes of unequal radii k_{Fa} and k_{Fb} and with a background reservoir of elec-

trons that are unaffected by the antiferromagnetism. We shall examine the changes in the antiferromagnetism with variation in the radii of the spheres which may be thought of as arising from either doping or from variations of the Fermi level with external parameters such as pressure, etc. If the electrons and hole spheres were equal in size, then the model would be just that discussed by Fedders and Martin[3] and would be mathematically equivalent to the BCS theory of superconductivity. Changing the relative sizes of the electron and the hole spheres is the mathematical equivalent to changing the Fermi radius for up spins relative to down spins in superconductivity. The effect of such a polarization on the superconducting transition has been studied extensively theoretically.[4-7] In the model for the antiferromagnetic (AF) transition, which we will discuss, there is an additional parameter, namely, the ratio of the density of states of the reservoir to that in the spheres, and there is complete mathematical equivalence between the two models only in the limit of an infinite density of states in the reservoir.

The energy spectra for the electron and hole pockets measured relative to the Fermi energy will be taken as

$$\begin{aligned}\epsilon^a(\vec{k}) &= v_F(k-k_{Fa}) = v_F(k-k_F)+H,\\ \epsilon^b(\vec{k}+\vec{Q}_0) &= -v_F(k-k_{Fb}) = -v_F(k-k_F)+H,\end{aligned} \tag{1}$$

where we define $k_F = \frac{1}{2}(k_{Fb}+k_{Fa})$ and $H = \frac{1}{2}v_F(k_{Fb}-k_{Fa})$ is the energy the Fermi level lies below for perfect nesting. The wave vector $\vec{Q}_0$ is the separation in reciprocal space between the centers of the electron (a) and hole (b) pockets and is determined by the band structure. We restrict ourselves to the weak-coupling limit, where H and the energy gap are much less than $v_F k_F$. We take a model Hamiltonian of the form

$$\mathcal{H} = \sum_{\vec{k}\sigma;\ a,b,c} \epsilon^a(\vec{k}) n^a_{\vec{k}\sigma} + \overline{V} \sum_{\vec{k}\vec{k}'\vec{q};\,\sigma\sigma'} a^\dagger_{\vec{k}+\vec{q}\sigma}\, a_{\vec{k}\sigma}\, b^\dagger_{\vec{k}'-\vec{q}\sigma'}\, b_{\vec{k}'\sigma'}\ , \tag{2}$$

where $a^\dagger$ and $b^\dagger$ are creation operators for electrons in the a and b pockets, respectively, n is the number operator, and $\overline{V}$ is the Fourier transform of the effective Coulomb interactions which we have taken as a constant. In choosing a Hamiltonian of form (2), we are ignoring the intraband exchange terms and all coupling between the magnetic portion of the Fermi surface (a and b bands) and nonmagnetic portion (c band). These approximations could influence the order of the transition that we find.

It is convenient to introduce the joint density of states function $N_{\vec{Q}_1}(\xi,\eta)$ defined as

$$\begin{aligned}N_{\vec{Q}_1}(\xi,\eta) = \sum_{\vec{k}} \delta(\xi - \tfrac{1}{2}[\epsilon^b(\vec{k}+\vec{Q}_1) - \epsilon^a(\vec{k})) \\ \times \delta(\eta - \tfrac{1}{2}[\epsilon^b(\vec{k}+\vec{Q}_1) + \epsilon^a(\vec{k}))\,.\end{aligned} \tag{3}$$

In this model it is straightforward to evaluate N and we find

$$N_{\vec{Q}_1,H}(\xi,\eta) = N_m Q^{-1}[\theta(\eta - H + Q) - \theta(\eta - H - Q)]\ , \tag{4}$$

where $Q = v_F\,|\,\vec{Q}_1 - \vec{Q}_0\,|$, $N_m = k_F^2/2\pi^2 v_F$, and $\theta(x)$ is the step function.

Let us study the Hamiltonian (2) in the Hartree-Fock approximation allowing for the possibility of antiferromagnetism. The AF state is characterized by nonzero expectation values of the form $\langle a^\dagger_{\vec{k},\sigma} \times b_{\vec{k}+\vec{Q}_1,-\sigma}\rangle$. Defining the order parameter $\Delta = \overline{V} \sum_{\vec{k}} \langle a^\dagger_{\vec{k},\sigma} b_{\vec{k}+\vec{Q}_1,-\sigma}\rangle$, we find the optimum value by minimizing the free energy with respect to Δ. This leads to the familiar gap equation

$$\begin{aligned}\Delta = \overline{V} \int d\xi\, d\eta\, N_{\vec{Q}_1,H'}(\xi,\eta)\,(\Delta/2E) \\ \times [1 - f(E+\eta) - f(E-\eta)]\ ,\end{aligned} \tag{5}$$

where $E^2 = \xi^2 + \Delta^2$, $f(\epsilon)$ in the Fermi function, and $H' - H$ is the shift in Fermi level in the AF state (see Fig. 1). Substituting from Eq. (4) and evaluating the right-hand side of Eq. (5) at $T = 0\,^\circ\mathrm{K}$, we arrive at the following equation for Δ:

$$-2\ln(\Delta/\Delta_0) = (\Delta/Q)[G(r_+) - G(r_-)]\ , \tag{6}$$

where

$$r_\pm = (Q \pm H')/\Delta,$$

$\Delta_0 = v_F k_F \exp(-1/N_m \overline{V})$ is the energy gap for $Q = H = 0$, and

$$\begin{aligned}G(x) &= x\cosh^{-1}x - (x^2-1)^{1/2}\,\mathrm{sgn}(x), && \text{for } |x| > 1\\ &= 0, && \text{for } |x| < 1.\end{aligned} \tag{7}$$

Equation (6) is identical to the gap equation of Fulde and Ferrell[6] for the analogous case of a superconductor in a strong exchange field.

The difference in the thermodynamic potential Ω between the paramagnetic and antiferromagnetic states at chemical potential μ is given by

$$\begin{aligned}\Omega_{AF}(\mu,Q,T) - \Omega_p(\mu,Q,T) &= \int_0^{\overline{V}} d(1/\overline{V})\,\Delta^2(\overline{V},Q,H') \\ &= -\int_0^{\Delta} \Delta^2 \left(\frac{\partial(1/\overline{V})}{\partial\Delta}\right) d\Delta.\end{aligned} \tag{8}$$

The optimum value of the $\vec{Q}$ vector is found by minimizing with respect to Q. This leads to the equation[6] for Q at $T = 0\,^\circ\mathrm{K}$,

$$Q^3 - \tfrac{3}{4}\Delta^2 Q[\gamma(r_+) + \gamma(r_-)] + \tfrac{1}{2}\Delta^3[\epsilon(r_+) + \epsilon(r_-)] = 0, \tag{9}$$

where $\gamma(x)$ and $\epsilon(x)$ are defined as follows:

$$\begin{aligned}\gamma(x) &= |x|\,(x^2-1)^{1/2} - \cosh^{-1}x, && |x| > 1\\ &\equiv 0, && |x| < 1,\\ \epsilon(x) &= \tfrac{3}{2}x\gamma(x) - \mathrm{sgn}(x)\,(x^2-1)^{3/2}, && |x| > 1\\ &\equiv 0, && |x| < 1.\end{aligned} \tag{10}$$

Finally, the position of the Fermi level in the antiferromagnetic phase H' is determined by the condition that the number of electrons is conserved. In Fig. 1, we show the single-particle energy bands in the antiferromagnetic phase. Equating the number of electrons removed from the paramagnetic reservoir with the number gained by the magnetic part, we get

$$N_p(H'-H) = 2N_m H - 2\int d\xi\, d\eta\, N_{\vec{Q},H'} \times [1-f(\eta-E)-f(\eta+E)], \tag{11}$$

where N_p is density of states per spin in the reservoir. Evaluating the right-hand side of Eq. (11) we get

$$(1+n)H - nH' = \tfrac{1}{4}\Delta^2 Q^{-1}[\gamma(r_+)-\gamma(r_-)]\ , \tag{12}$$

where $n = N_p/2N_m$ denotes the ratio of the density of states of the reservoir to the magnetic part of the surface.

The three coupled Eqs. (6), (9), and (12) determine the values of Δ, Q, and H' as a function of H, the Fermi level in the paramagnetic state. If for a given value of H there is more than one solution, then the solution with the lowest energy is the physical one.

Let us restrict our attention first to $Q \equiv 0$. Then, the equations simplify considerably. In the limit $n \to 0$, there is only one nontrivial solution

$$\Delta^2 = \Delta_0(\Delta_0 - 2H) \tag{13}$$

shown in Fig. 2 as a function of H. This solution clearly gives a second-order transition at $H = \Delta_0/2$, where Δ_0 is the BCS value when $H = 0$, $T = 0$ °K. However, in the opposite limit $n \to \infty$, $H' \equiv H$ and we find two solutions in addition to the trivial paramagnetic solution $\Delta \equiv 0$, [4,5]

$$\Delta = \Delta_0, \qquad H < \Delta_0 \tag{14a}$$

$$\Delta^2 = \Delta_0(2H - \Delta_0), \quad \tfrac{1}{2}\Delta_0 < H < \Delta_0. \tag{14b}$$

By examining the ground-state energy E_G, it is straightforward to show that (14b) is unphysical and that there is a first-order transition between the fully polarized state, (14a), and the paramagnetic state $\Delta \equiv 0$ at $H = \Delta_0/\sqrt{2}$. As n increases from zero, one finds a second-order transition for $n < 1$ and first-order one for $n > 1$.

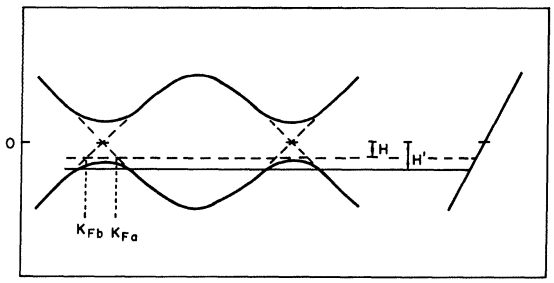

FIG. 1. Band structure in the unequal sphere model. The b pocket centered at $\vec{Q}_1$ has been mapped onto the origin and the zero of energy has been chosen as shown.

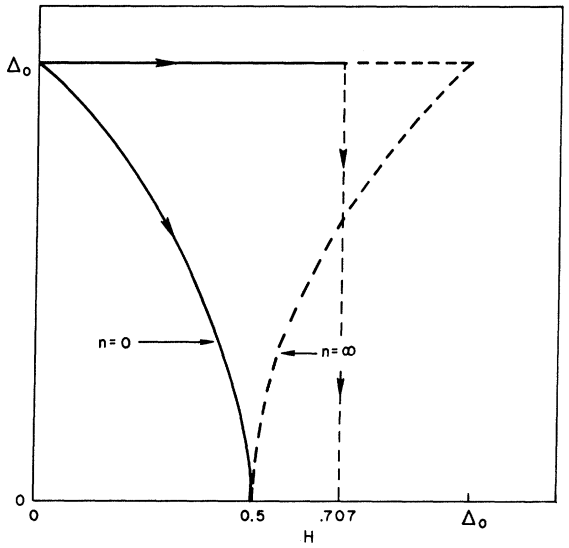

FIG. 2. Solutions of the gap equation at $T = 0$ °K for $Q \equiv 0$. The heavy dashed line denotes the unphysical region.

At finite temperatures we may proceed through an analogous series of calculations. In the limit $H \to 0$, the model reduces identically to the Fedders-Martin (BCS) model. In this limit the antiferromagnetic to paramagnetic transition at T_N^0 is clearly second order. In the region $n < 1$, the transition at $T = 0$ °K with increasing H is also second order. One finds that for all intermediate values of H the transition which now occurs at finite temperature is second order. For $n > 1$, however, the transition at $T = 0$ °K with increasing H is first order. For $n > 1$, one finds that for small values of H the transition remains second order, but for the large values of H (less than the critical value) the transition with increasing temperature is first order. Thus, for any $n > 1$, there is a critical value of H or equivalently of T_N, such that for $T_N > T_N^c$, the transition is second order and for $T_N < T_N^c$, the transition is first order. In the limit $n \to \infty$, this critical value $T_N^c = 0.55 T_N^0$. [4,5]

The situation changes considerably when we relax the condition $Q \equiv 0$. First, let us calculate the right-hand side of the gap equation (5) in the limit $\Delta \to 0$. The right-hand side is proportional to the band susceptibility $\chi_0(Q)$ defined as

$$\chi_0(Q) = -\sum_{\vec{k}} \frac{f(\epsilon^b_{\vec{k}+\vec{Q}_1}) - f(\epsilon^a_{\vec{k}})}{\epsilon^b(\vec{k}+\vec{Q}_1) - \epsilon^a(\vec{k})} \tag{15}$$

$$= \int d\xi\, d\eta\, N_{\vec{Q}_1,H}(\xi,\eta)\,(2\xi^{-1})[1-f(\xi+\eta)-f(\xi-\eta)] \tag{16}$$

$$= N_m\left[\tfrac{1}{2}\ln\left(\frac{v_F^2 k_F^2}{2(Q^2-H^2)}\right)+1-\frac{H}{2Q}\ln\left|\frac{Q+H}{Q-H}\right|\right]. \tag{17}$$

In Fig. 3, we plot $\chi_0(Q)$ at $T=0$ °K as a function of Q. We see at once that the maximum occurs not at $Q=0$ but at $Q\simeq 1.2H$. Thus, if the paramagnetic to AF transition is second order as H increases at 0 °K, then it must occur with $Q\simeq 1.2H$. Substituting this value of Q into the right-hand side of Eq. (6), we find that the critical value of H for a second-order transition is $H=0.753\Delta_0$. Note this value is independent of n. The paramagnetic reservoir plays a role only at a first-order transition where finite repopulation effects can occur. The paramagnetic-antiferromagnetic transition occurs first as a second-order transition to a finite Q state for all values of n. In this model the finite Q state is the analog of the Fulde-Ferrell state[6] for superconductors in the presence of a strong exchange field.

In the limit $n\to\infty$, Eq. (12) reduces simply to $H'\equiv H$. In this limit there is complete mathematical equivalence with superconductivity in a strong exchange field. If we plot Δ as a function of H, then, following Fulde and Ferrell,[6] we get a curve of the form shown in Fig. 4. There is a first-order phase change at H slightly less than $0.71\Delta_0$ from the $Q=0$ or $\vec{Q}_1=\vec{Q}_0$ AF phase to an AF state with $Q\simeq 0.9\Delta_0$. This discontinuous change in $\vec{Q}$ vector as a function of an external variable was predicted on general grounds by Herring.[9] Subsequently, Falicov and Penn studied such a first-order transition in a model which is similar to that under consideration here.[10] The commensurate-incommensurate phase change observed in some Cr alloys[8] is an example of such

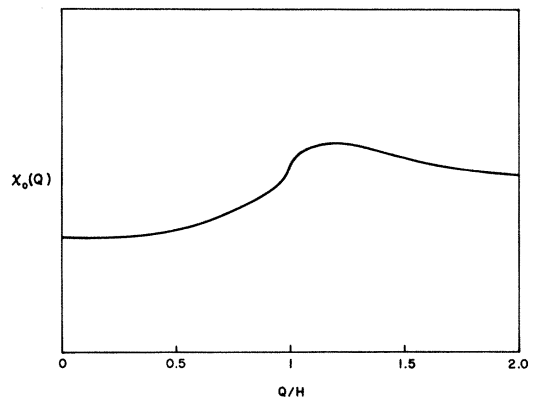

FIG. 3. Band susceptibility in the unequal sphere model at $T=0$ °K.

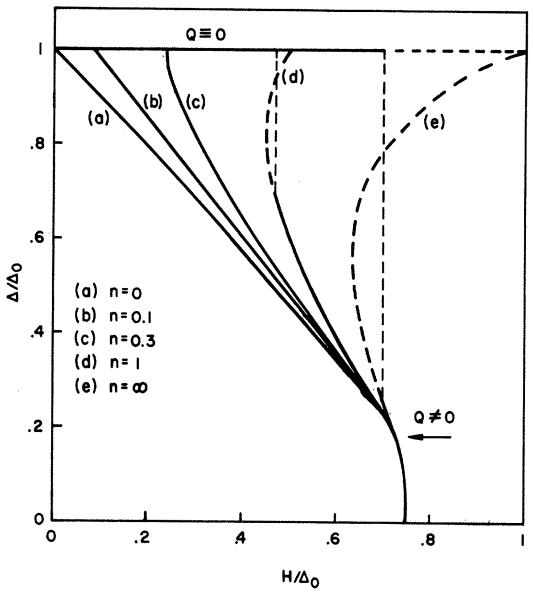

FIG. 4. Solutions of the gap equation at $T=0$ °K for various values of n. The heavy dashed line denotes the unphysical region.

an effect. In pure Cr the electron and hole pockets are unequal in size with the body of electron jack smaller than the hole octahedron. The Q vector of the antiferromagnetic phase is approximately $0.96(\vec{G}/2)$, where $\vec{G}$ is a (1, 0, 0) reciprocal-lattice vector. On alloying with Mn, Ru, Re, etc., to increase the electron-to-atom ratio and therefore the electron pocket relative to the hole pocket, an abrupt jump in Q vector is found to the commensurate value $Q=\frac{1}{2}\vec{G}$.

However, if we take the opposite limit of $n\to 0$, i.e., no paramagnetic reservoir, then we find the solution of Eqs. (6), (9), and (12) is single valued as shown in Fig. 4. Thus, in this limit the $\vec{Q}$ vector varies continuously away from $\vec{Q}_1=\vec{Q}_0$, as H increases from zero. Note that we have omitted the higher-order terms which Herring[9] showed lead to a discontinuity in Q vector. For a general value of n, the solution is complicated. We have solved numerically the set of Eqs. (6), (9), and (12) for various values of n. The results obtained for $\Delta(H)$ are shown in Fig. 4. For $n\leq 0.31$, we find that $\Delta(H)$ is single valued. For $H<n\Delta_0/(1+n)$, we find $Q\equiv 0$ and for $H>n\Delta_0/(1+n)$, $Q\neq 0$. The transition between the commensurate ($Q\equiv 0$) and incommensurate ($Q\neq 0$) phase is continuous and second order. However, for values of $n>0.31$, the curves for $\Delta(H)$ are multivalued as shown in Fig. 4. This leads to a first-order transition between the commensurate and incommensurate phases as H is increased.

In Cr the density of states is approximately halved

on going through the AF transition[15] which leads to value of $n \approx 1$ and a first-order commensurate-incommensurate transition even without the higher-order terms which Herring[9] included. In the commensurate phase the energy gap Δ is constant, independent of H and T_N. At the first-order phase transition it drops abruptly to a value $\approx 0.7\Delta_0$ and varies continuously to zero as H is increased. These results are in qualitative agreement with those of Barker and Ditzenberger,[16] who find a value of the gap which is roughly constant in the commensurate phase of various Cr alloys. In the incommensurate phase on the other hand they find that Δ varies approximately linearly with T_N. The model band structure is too crude to allow us to make a quantitative comparison with experiment.

Lastly, we consider the properties of the system near the Néel temperature. As we stressed earlier, if the transition is second order, the existence of a reservoir does not affect the Néel temperature. We can then obtain the dependence of the transition temperature on H from the calculations in the analogous problem in superconductivity by Saint-James and Sarma.[7] Their results are shown as the solid line in Fig. 5. Furthermore, using the superconductivity results we see that in the $n \to \infty$ limit, the paramagnetic to AF transition is, in fact, second order. For $H < 0.707\Delta_0$ and equivalently $T_N > T_N^c = 0.55T_n^0$, the transition at the Néel temperature is initially to a $Q \equiv 0$ or $\vec{Q}_1 \equiv \vec{Q}_0$ state, and for $0.707\Delta_0 < H \lesssim 0.75\Delta_0$, the transition is to a finite Q state. Since the transition at the Néel temperature is second order in both $n = 0$ and $n = \infty$ limits, we believe that this transition will remain second order for all values of n. It then follows that the value of T_N is the same as in the case $n = \infty$ for a given value of H. For some values of H and n, there will also be transition between an AF state with $Q \equiv 0$ and one with finite Q. The transition temperature and also the order of this transition will depend on n and H.

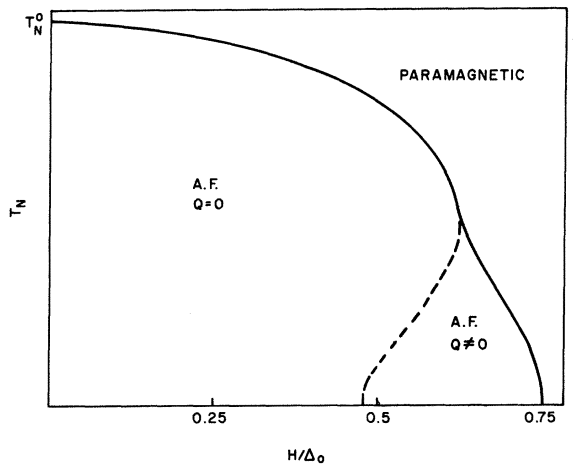

FIG. 5. Néel temperature versus H. The dashed line denotes the transition temperature of the commensurate-incommensurate transition for $n = 1$.

The dashed line in Fig. 5 is the locus of this transition for $n = 1$, the value appropriate to Cr. The point where the $Q \equiv 0$ to $Q \neq 0$ transition curve meets the curve of T_N is independent of n, and there is a discontinuity in the second derivative of $T_N(H)$ at this point. The foot of the curve is at a value of H where the commensurate-incommensurate transition occurs in Fig. 4. A final feature of interest is the curve of T_N versus H in the region near $H_c = 0.75\ \Delta_0$, where $T_N \to 0$. The curve has a square-root behavior $T_N \sim (H_c - H)^{1/2}$ in this region.

III. CUSP-TYPE KOHN SINGULARITY

In Sec. II, we discussed a model with a band susceptibility which had a regular maximum. We now wish to examine the question of how the existence of singular maxima in the band susceptibility $\chi_0(q)$ can influence the transition. We will consider in this section the case of a cusp-type Kohn singularity in the susceptibility. The possibility of cusps in the susceptibility was first demonstrated by Roth, Zeiger, and Kaplan.[13] These authors showed that if for a given value of $\vec{Q}$, say $\vec{Q}_0$, a curve of intersection between the Fermi surface and the Fermi surface displaced by $\vec{Q}_0$ crosses itself at a point, then there will be a cusp in $\chi_0(\vec{Q})$ at $\vec{Q} = \vec{Q}_0$, at 0 °K.

The wave-vector-dependent susceptibility $\chi(\vec{Q})$ in the generalized random-phase approximation is given by

$$\chi(\vec{Q}) \sim \chi_0(\vec{Q})/[1 - \bar{V}\chi_0(\vec{Q})], \tag{18}$$

where $\chi_0(\vec{Q})$ is the generalized band susceptibility introduced in Eq. (15). At a second-order transition to an antiferromagnetic transition, $\chi(\vec{Q}) \to \infty$. Clearly, as we vary $\bar{V}$ by varying some external parameters such as pressure, the transition will occur first at a maximum of $\chi_0(\vec{Q})$. We shall take a simple model band structure which exhibits a cusp-type singularity; we shall assume that $\chi_0(\vec{Q})$ attains its maximum value at the apex of this cusp and examine the nature of the AF transition as we vary $\bar{V}$.[17]

We begin by considering a band structure of the form

$$\epsilon^b(\vec{k} + \vec{Q}_0) = vk_z + \frac{k_x^2}{2m_x} - \frac{k_y^2}{2m_y}\ ,$$
$$\epsilon^a(\vec{k}) = -vk_z + \frac{k_x^2}{2m_x} - \frac{k_y^2}{2m_y}\ . \tag{19}$$

Let us examine the curves of intersection of the two surfaces $\epsilon^a(\vec{k}) = 0$ and $\epsilon^b(\vec{k} + \vec{Q}) = 0$ as we vary $\vec{Q}$ through the value $\vec{Q}_0$. Denoting the product $v(Q - Q_0)_z$

by q we find that for $q>0$ the curves of intersection lie in the (k_x, k_y) plane and form a hyperbola as shown in Fig. 6(a). The shaded area denotes the region where the perpendicular distance to the b surface k_z^b is greater than the distance to the a surface k_z^a. As q varies through zero, the branches of the hyperbola approach each other along the k_y axis, touch at $q=0$, and then separate along the k_x axis. The joint density of states defined in (3) $N_{\vec{Q}}(\xi, \eta)$ can be evaluated at once for this model and we find

$$N_{\vec{Q}}(\xi, \eta)=\sum_{\vec{k}} \delta(\xi - v k_z - \tfrac{1}{2}q)\delta\left[\eta-\left(\frac{k_x^2}{2m_x}-\frac{k_y^2}{2m_y}\right)-\tfrac{1}{2}q\right] \tag{20}$$

$$=\nu_0 \ln\left|\eta_0/(\eta-\tfrac{1}{2}q)\right|, \tag{21}$$

where η_0 is a cutoff energy in the (k_x, k_y) plane and $\nu_0 = (m_x m_y)^{1/2}/4\pi^3 v$. For $q=0$ or $\vec{Q}=\vec{Q}_0$, N has a logarithmic divergence as $\eta \to 0$. This in contrast to the behavior at a usual type of Kohn anomaly which causes a discontinuous jump in the value of $N_Q(\xi, \eta)$. In the model discussed in Sec. II, there is an ordinary Kohn singularity at $Q=\pm H$ and associated with it is a discontinuity in N [see Eq. (4)].

The gap equation for general band structure can be written in the form

$$1/\overline{V}=A(q, \Delta, T) \tag{22}$$

$$=\int d\xi\, d\eta\, N_{\vec{Q}}(\xi, \eta)\,(2E)^{-1}[1-f(E+\eta)-f(E-\eta)]. \tag{23}$$

From knowledge of the function A, we can readily determine the order of the transition in the Hartree-Fock approximation. By the particle-hole symmetry of our model, the Fermi level in the AF phase will be the same as in the paramagnetic phase.

We can rewrite Eq. (8) as

$$\Omega_{AF}-\Omega_p=\int_0^{\Delta}\frac{dA}{d\Delta}(\Delta, q, T)\Delta^2 d\Delta, \tag{24}$$

where Δ is the value which satisfies Eq. (22). Consider now if the maximum of A as a function of Δ occurs at $\Delta=0$ for all q and T, then $dA/d\Delta \le 0$ for small Δ and the transition is clearly second order. On the other hand, suppose that for temperatures near the transition the maximum of A with respect to q and Δ occurs away from $\Delta=0$ at $\Delta=\Delta_m(T)$. Then as the temperature is reduced we first get a solution of Eq. (22) with $\Delta=\Delta_m$. Clearly, $dA/d\Delta>0$ as we go from $\Delta=0$ to $\Delta=\Delta_m$ and the integral (24) is positive. Therefore, the paramagnetic free energy is lower. As we lower T further, there are two solutions with $\Delta>\Delta_m(T)$ and $\Delta<\Delta_m(T)$, respectively. If we take the solution with $\Delta>\Delta_m$, there are both positive and negative contribution to the integral (24) and the value of the integral is always less than that which would have resulted from the choice of the other solution for Δ. The transition occurs when the integral (24) equals zero and the state of lowest free energy changes discontinuously from a state with $\Delta=0$ to one with a value $\Delta>\Delta_m(T)$ and the transition is, therefore, first order.

We will now proceed to examine the gap equation in the model band structure described by Eq. (19). Substituting from Eq. (21) and evaluating the right-hand side at $T=0$ °K, we get

$$A(q, \Delta)=\nu_0\int_{-\omega_0}^{\omega_0} d\xi \frac{1}{2E}\int_{-E}^{E} d\eta \ln\left|\frac{\eta_0}{\eta-\frac{1}{2}q}\right|$$

$$=\nu_0\int_{-\eta_0}^{\eta_0} d\xi\left(\ln\eta_0+\frac{\frac{1}{2}q}{2E}\ln\left|\frac{E-\frac{1}{2}q}{E+\frac{1}{2}q}\right|\right.$$

$$\left.-1-\tfrac{1}{2}\ln\left|\tfrac{1}{4}q^2-E^2\right|\right)+2\nu_0\int_{\eta_0}^{\omega_0} d\xi \ln\eta_0, \tag{25}$$

where ω_0 is the upper cutoff on the ξ integration.

Expanding the right-hand side as a function of Δ and q we find

$$A(q, \Delta)=A_0-\alpha[(\Delta^2-\tfrac{1}{4}q^2)^{1/2}-\tfrac{1}{2}q\sin^{-1}(\tfrac{1}{2}q/\Delta)]$$

$$+0(\Delta/\eta_0, \Delta/\omega_0), \quad \Delta>\tfrac{1}{2}q \tag{26}$$

$$=A_0-\tfrac{1}{4}\alpha\pi\left|q\right|+0(q/\eta_0, q/\omega_0), \quad \Delta<\tfrac{1}{2}q \tag{27}$$

where A_0 and α are constants:

$$A_0=\nu_0[4\eta_0+2\eta_0\ln(\omega_0/\eta_0)], \quad \alpha=\pi\nu_0. \tag{28}$$

Examining the results first in the limit $\Delta \to 0$, we see that $A(q, 0)$ has a cusp centered at $q=0$. This cusp is a reflection of the cusp-type Kohn anomaly in $\chi_0(\vec{Q})$ derived by Roth *et al.*[13] In Fig. 7, we plot $A(q, \Delta)$. The maximum value of A occurs at $\Delta=0$, $q=0$. Thus, as A_0 varies through $\overline{V}^{-1}$ at 0 °K, there will be a second-order transition between a paramagnetic state and an AF state with $q=0$ or $\vec{Q}=\vec{Q}_0$. The linear dependence of $A(0, \Delta)$ on Δ will give rise to a linear dependence of Δ on external parameters in contrast to the square-root depen-

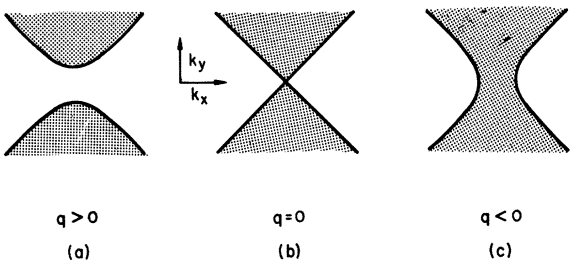

FIG. 6. Curves of intersection of the Fermi surfaces $\epsilon^a(\vec{k})=0$ and $\epsilon^b(\vec{k}+\vec{Q})=0$ given by Eq. (19).

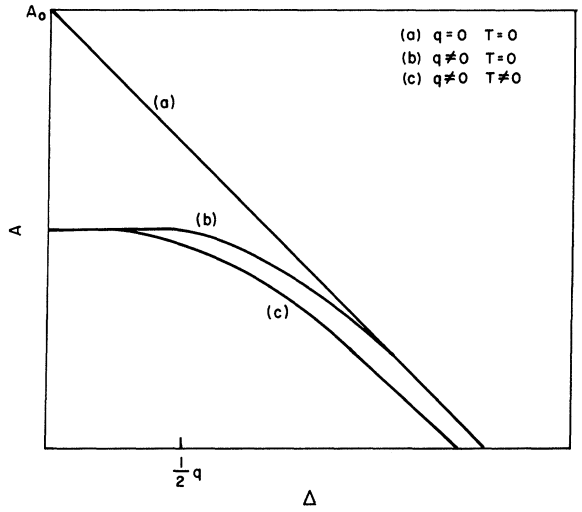

FIG. 7. Function $A(q, \Delta, T)$ plotted against Δ for various choices of q and T.

dence which was found in Sec. II. The square-root dependence is characteristic of a transition that occurs at a *regular* maximum in $\chi_0(\vec{Q})$.

A first-order transition will occur if the function $A(q, \Delta)$ has its maximum value at a finite value of Δ. It is possible to obtain this condition by introducing strong-coupling corrections and additional contributions from other bands. Let us divide $\chi_0(\vec{Q})$ into two parts $\chi_0 = \chi_0' + \chi_0''$, where χ_0' is the nonanalytic contribution calculated above and χ_0'' is a background analytic contribution from the nonmagnetic bands. Then we have

$$\frac{d\chi_0}{dq} = -\frac{\pi^2}{4}\nu_0 \operatorname{sgn}(q) + \frac{d\chi_0''}{dq} \ . \tag{29}$$

In general $d\chi_0''/dq \neq 0$ for $q = 0$, thus, by a suitable choice of χ_0'', we can make $d\chi_0/dq$ as small as we like for $q < 0$. Under these circumstances strong-coupling corrections can lead to a first-order transition. In the weak-coupling limit, $A(q, \Delta)$ is a constant as a function of Δ for $\Delta < \frac{1}{2}q$. However, the terms of order $0(\Delta/N_0, \Delta/\omega_0)$ may be increasing functions of Δ as we increase Δ away from zero. We have calculated these terms numerically for the model band structure in (19) and we find that they can cause a maximum in $A(q, \Delta)$. The value of this maximum clearly depends on the model band structure. However, by a suitable choice of parameters, it is possible to simultaneously satisfy the conditions that $\max\{A(q, 0)\}$ is at $q = 0$ and $\max\{A(q, \Delta)\}$ is at $\Delta \neq 0$ and $q \neq 0$, leading to first-order transition at $T = 0\,^\circ\mathrm{K}$ as $\bar{V}$ is varied.

At finite temperatures, the step function in Eq. (23) is replaced by the Fermi function. Because of the exponential character of the Fermi function, we have not found it possible to carry out the necessary integrations analytically. Therefore, we replaced the Fermi function at finite temperature by a slanting function (see Fig. 8) defined as

$$\begin{aligned} f(\epsilon) &= 1, \quad \epsilon < -CT, \quad k_B \equiv 1 \\ &= \tfrac{1}{2}[1 - (\epsilon/CT)], \quad -CT < \epsilon < CT \\ &= 0, \quad \epsilon > CT \end{aligned} \tag{30}$$

where C is a constant which we choose equal to 2.7 for reasons to be discussed below. With this approximation it is possible to carry out all integrations analytically.

Let us first evaluate A with $\Delta \equiv 0$. We find after some algebra

$$A(q, 0, T) = A_0 - \tfrac{1}{4}\alpha\pi(2CT)^{-1}[(CT - \tfrac{1}{2}q)^2 \times \operatorname{sgn}(CT - \tfrac{1}{2}q) + (CT + \tfrac{1}{2}q)^2 \operatorname{sgn}(CT + \tfrac{1}{2}q)] \tag{31}$$

$$\sim A_0 - \tfrac{1}{4}\alpha\pi CT, \quad CT > \tfrac{1}{2}q \tag{32}$$

$$= A_0 - \tfrac{1}{4}\alpha\pi \left| q \right|, \quad \tfrac{1}{2}q > CT \ . \tag{33}$$

The effect of the finite temperature is to round the cusp in $A(q, 0, 0)$ or $\chi_0(q)$. For small q, the maximum height drops linearly with increasing temperature, while away from the apex of the cusp the temperature causes only very small changes. The linear dependence on T causes a linear dependence of the critical temperature for a second-order transition on external parameters in the limit $T_N \to 0$. The experiments of McWhan[18] on the pressure dependence of T_N in Cr-V and Cr-Mo alloys support such a linear dependence for the antiferromagnetism of Cr.

A numerical evaluation of $A(0, 0, T)$ using the Fermi function gives

$$A(0, 0, T) = A_0 - 2.1\ \alpha T \ . \tag{34}$$

The constant C was chosen so that the linear coefficient in the "slanting" approximation expansion

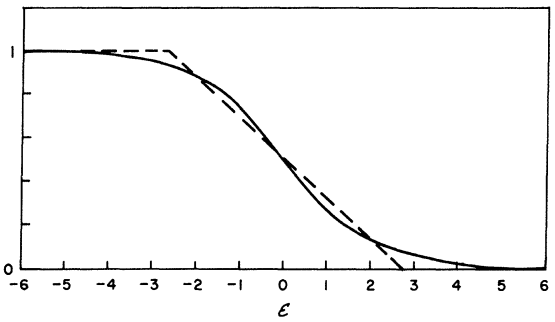

FIG. 8. Fermi function (solid curve) and the slanting approximation to it (dashed curve).

(32) would equal that in the exact expansion (34).

For a more general band structure with a cusp-type Kohn anomaly, the coefficient α can be expressed following Roth, Zeiger, and Kaplan[13] in terms of v_{z1} and v_{z2}, the perpendicular velocities in the two bands, and κ_{xx} and κ_{yy}, the parameters of the hyperbolas of intersection between the electron and hole pockets. As $\vec{Q}$ varies through $\vec{Q}_0$, the family of hyperbolas of intersection is given by

$$(\vec{Q}-\vec{Q}_0)_z = -\tfrac{1}{2}(\kappa_{xx}k_x^2+\kappa_{yy}k_y^2). \tag{35}$$

We then find for a general band structure using the slanting approximation to the Fermi functions

$$\begin{aligned} A(q_z,\ 0,\ T) = A_0 &- (16\pi\,|\,\kappa_{xx}\kappa_{yy}\,|^{1/2}\,|\,v_{z1}v_{z2}\,|\,b^2CT)^{-1} \\ &\times[(q_z'+CbT)^2\,\mathrm{sgn}(q_z'+CbT) \\ &-(q_z'-CbT)^2\,\mathrm{sgn}(q_z'-CbT)], \end{aligned} \tag{36}$$

where $q_z' = (Q-Q_0)_z$ and $b = |\,v_{z1}-v_{z2}\,|/|\,v_{z1}v_{z2}\,|$.

Finally, we evaluate $A(q,\ \Delta,\ T)$ as a function of all three variables for the simple band structure using the slanting approximation to the Fermi functions. After some algebra we find

$$\begin{aligned} A(q,\ \Delta,\ T) = A_0 - \frac{\nu_0}{\pi}\Bigg(&\frac{t_+^2}{8T}F_1(t_+,\Delta)+\frac{t_-^2}{8T}F_1(t_-,\Delta) \\ &+\frac{1}{4CT}\{F_2(t_+,\Delta)+F_2(t_-,\Delta) \\ &+\tfrac{1}{2}[t_+F_3(t_+,\Delta)+t_-F_3(t_-,\Delta)]\}\Bigg), \end{aligned} \tag{37}$$

where $t_\pm = CT \pm \frac{1}{2}q$ and three functions F_1, F_2, and F_3 are defined as follows:

$$\begin{aligned} F_1(t,\Delta) &= \int_0^{\omega_0}\frac{d\xi}{E}\ln\left|\frac{t+E}{t-E}\right| \\ &= \pi\sin^{-1}t/\Delta, && \Delta > |\,t\,| \\ &= \tfrac{1}{2}\pi^2\,\mathrm{sgn}(t), && \Delta < |\,t\,| \end{aligned} \tag{38}$$

$$\begin{aligned} F_2(t,\Delta) &= -\int^{\omega_0} d\xi\left(t\ln\left|\frac{t-E}{t+E}\right|-2t\right) \\ &= -\tfrac{1}{2}\pi t(\Delta^2-t^2)^{1/2}+\tfrac{1}{2}\pi\Delta^2\sin^{-1}(t/\Delta), && \Delta > |\,t\,| \\ &= \tfrac{1}{4}\pi^2\Delta^2\,\mathrm{sgn}(t), && \Delta < |\,t\,| \end{aligned} \tag{39}$$

and

$$\begin{aligned} F_3(t,\Delta) &= \int_0^{\omega_0} d\xi\ (\ln|\,t^2-E^2\,|-2\ln\xi) \\ &= \pi(\Delta^2-t^2)^{1/2}, && \Delta > |\,t\,| \\ &= 0, && \Delta < |\,t\,|. \end{aligned} \tag{40}$$

In each case we have kept only the leading terms in Δ and t and ignored corrections of order $(\Delta/\omega_0,\ t/\omega_0)$. In Fig. 7, we plot A as a function of Δ in the region $CT < |\,\frac{1}{2}q\,|$. In this region, $A(\Delta)$ is constant up to $\Delta = \frac{1}{2}q - CT$ and then falls off. It is clear that this feature is a result peculiar to the slanting approximation, and if we had used the full Fermi function, then A would monotonically decrease as a function of Δ. In the limit when $CT > \frac{1}{2}q$, A is also a monotonically decreasing function of Δ and T. Thus, in this simple model we find that there is always a second-order transition.

We showed earlier that the contribution from other bands could cause a first-order transition at $T = 0\ ^\circ\mathrm{K}$. Since the nonanalytic contributions at $T = 0\ ^\circ\mathrm{K}$ to A always fall off monotonically as T increases from $0\ ^\circ\mathrm{K}$ and, further, fall off faster at finite Δ and q than at $\Delta = 0$ and $q = 0$, it is clear that by increasing the coupling we will convert the first-order transition at $T = 0\ ^\circ\mathrm{K}$ to a second-order transition when the Néel temperature T_N exceeds a critical value T_N^c, depending on the parameters of the model.

Recently, Kimball and Falicov[19,20] have examined the paramagnetic to antiferromagnetic phase change in a model with a single tight binding s band hydridised with a plane-wave band. For this model, they find in the Hartree-Fock approximation at finite temperatures a first-order paramagnetic to antiferromagnetic phase transition. However, at $T = 0\ ^\circ\mathrm{K}$ the transition is second order as the coupling constant is varied through its critical value. The Néel temperature appears to go to zero linearly with coupling strength, while the ratios of the zero-temperature energy gap and of the extrapolated second-order transition temperature from below to T_N remain constant. This latter behavior suggests that the peak in χ_0, the one-electron-band susceptibility for their model, is at a cusp-type Kohn anomaly. An examination in detail of their band structure shows that it has a cusp-type Kohn anomaly at approximately the correct position. It is not clear from their numerical calculation which feature of their model is responsible for the difference in behavior between their model and the results we have obtained above.

IV. MORE GENERAL KOHN ANOMALIES

In Sec. III, we discussed the case of a cusp-type maximum in the susceptibility which occurs if the point of tangency is at the intersection of two lines of intersection. It is possible for more complicated anomalies to occur. Thus, for example, one could have at a symmetry point several lines of intersection, crossing at a point of tangency. It is straightforward to generalize the analysis of Roth *et al.*[12] to cover this case. One finds at $T = 0$ a nonanalytic contribution to $\chi_0(q)$ of the form $-B\,|\,q\,|^{2/n}$, where n is the number of lines of intersection crossing at the point of tangency. The model band structure discussed in Sec. III corresponds to the case $n = 2$. It is straightforward to generalize the calculation of the temperature dependence, at least in the slanting approximation, and one finds that the sus-

ceptibility at $q = b$ behaves like $-cT^{2/n}$ near $T = 0$.

Other forms of the singularity are mathematically possible. One example is the cylindrical anomaly discussed by Roth *et al.*[13] which will occur if at critical contact there is a line of tangency rather than a point of tangency. Another example, is perfect nesting where critical contact occurs simultaneously over a plane of tangency. Neither of these examples will occur precisely in nature, but it is, nonetheless, interesting to analyze these models since they may represent useful approximations to actual physical systems over limited regions of temperature, etc. The analysis of the perfect nesting example is similar to the BCS model of superconductivity and leads, of course, to well-known results and, in particular, a second-order transition.[3]

In this section, we shall analyze a model of the cylindrical type. We choose

$$\epsilon^a_{\vec{k}} = k_x^2/2m + Vk_z \ , \qquad \epsilon^b_{\vec{k}+\vec{Q}} = k_x^2/2m - V(k_z + q_z') \ , \tag{41}$$

where, again, we have chosen the k_z direction perpendicular to the plane of tangency and $q_z' = (Q - Q_0)_z$. At $q_z' = 0$, the two surfaces are tangent along the y axis. It is straightforward, for this model, to evaluate $N_{\vec{Q}}(\xi, \eta)$ defined in (3) and we find

$$N_{\vec{Q}}(\xi, \eta) = \frac{L(2m)^{1/2}}{8\pi^3 V} \frac{\theta(\eta - \frac{1}{2}Vq_z')}{(\eta - \frac{1}{2}Vq_z')^{1/2}} \ , \tag{42}$$

where L is the length of the line of tangency. At a cylindrical anomaly, $N_{\vec{Q}}$ has a square-root divergence at the origin. If we substitute this form in the general formula for $A(q_z', \Delta, T)$, then, after some algebra, we find at $T = 0\,^\circ\mathrm{K}$ that

$$A(q_z', \Delta, T=0) = \frac{L(2m)^{1/2}}{8\pi^3 V} \int_{-\eta_0}^{\eta_0} d\eta \frac{\theta(\eta + \frac{1}{2}Vq_z')}{(\eta + \frac{1}{2}Vq_z')^{1/2}} \times \int_{-\omega_0}^{\omega_0} \frac{d\xi}{2E}[1 - f(E+\eta) - f(E-\eta)] \tag{43}$$

$$= \frac{L(2m)^{1/2}}{8\pi^3 V} \int_{-\eta_0}^{\eta_0} d\eta \frac{\theta(\eta + \frac{1}{2}Vq_z')}{(\eta + \frac{1}{2}Vq_z')^{1/2}} \times \ln\left(\frac{\omega_0 + (\omega_0^2 + \Delta^2)^{1/2}}{|\eta| + (\eta^2 + \Delta^2)^{1/2}} \right) . \tag{44}$$

We have not evaluated this integral in general but will examine the behavior in certain limits. First, in the limit $\Delta \to 0$ we find

$$A = \frac{L(2m)^{1/2}}{8\pi^3 V} \int_{-\eta_0}^{\eta_0} d\eta \frac{\theta(\eta + \frac{1}{2}Vq_z')}{(\eta + \frac{1}{2}Vq_z')^{1/2}} \left(\ln \frac{\omega_0}{|\eta|} - \frac{\Delta^2}{4\eta^2} + \cdots \right) \tag{45}$$

$$= A_0 - \frac{Lm^{1/2}}{4\pi^2 V}(-Vq_z')^{1/2}\left(1 + \frac{\Delta^2}{(Vq_z')^2} + \cdots\right) \ , \quad Vq_z' < 0 \tag{46}$$

$$= A_0 + 0\left(\frac{Vq_z'}{\eta_0}, \frac{\Delta}{\eta_0}\right) , \qquad Vq_z' > 0 \tag{47}$$

where

$$A_0 = [L(2m\eta_0)^{1/2}/4\pi^3 V][\ln(\omega_0/\eta_0) + 2]. \tag{48}$$

The square-root singularity in $A(q_z', 0, 0)$ is the cylindrical anomaly found by Roth, Zeiger, and Kaplan.[13] In the opposite limit $\Delta \gg |Vq_z'|$, we can expand Eq. (44) and we find

$$A = \frac{L(2m)^{1/2}}{8\pi^3 V}\left[\int_0^{\eta_0} \frac{d\eta}{\eta^{1/2}} \ln\left(\frac{\omega_0 + (\omega_0^2 + \Delta^2)^{1/2}}{\eta + (\eta^2 + \Delta^2)^{1/2}}\right) + \tfrac{1}{2}Vq_z' \int_0^{\eta_0} \frac{d\eta}{\eta^{1/2}(\eta^2 + \Delta^2)^{1/2}} + \cdots\right] \tag{49}$$

$$= A_0 + \frac{L(2m)^{1/2}}{8\pi^3 V} \int_0^{\eta_0} d\eta \left[\left(\frac{\eta^{1/2}}{(\eta^2 + \Delta^2)^{1/2}} - 1\right) + \frac{\frac{1}{2}Vq_z'}{\eta^{1/2}(\eta^2 + \Delta^2)^{1/2}} + \cdots\right] . \tag{50}$$

These latter integrals may be evaluated in terms of elliptic functions and we find

$$A = A_0 - 0.84 \frac{L(2m\Delta)^{1/2}}{4\pi^3 V}\left(1 - 1.1\frac{Vq_z'}{\Delta} \cdots\right) . \tag{51}$$

Examining A as a function of Δ at various values of q_z', we see at once that A is a monotonically decreasing function of Δ with its maximum value at the origin. Thus, at $T = 0\,^\circ\mathrm{K}$, the transition is second order.

Finally, we estimate the temperature smearing of the square-root singularity of the susceptibility. Again, we have recourse to the slanting approximation. After some algebra we obtain

$$A(q_z', \Delta = 0, T) = A_0 - [L(2m)^{1/2}/24\pi^2 V] \times [(2CT - \tfrac{1}{2}Vq_z')^{3/2}\theta(2CT - \tfrac{1}{2}Vq_z') - (-2CT - \tfrac{1}{2}Vq_z')^{3/2}\theta(-2CT - \tfrac{1}{2}Vq_z')] . \tag{52}$$

The effect of temperature is to smear out the square-root singularity. The apex at $q_z' = 0$ drops initially as $T^{1/2}$. Away from the apex, the falloff is much slower. Although we have only calculated at $T = 0$ and finite Δ, and $\Delta = 0$ and finite T, there is nothing to suggest that raising the temperature could change a second-order transition to a first-order one. Thus, the occurrence of a Kohn anomaly does not lead to a first-order transition, but does lead to anomalous

dependences of T_N and Δ in the limit of low temperatures.

V. CONCLUSIONS

In this paper, we have examined the effects of imperfect nesting of the band structure on itinerant antiferromagnetism. In Sec. II, we studied a model in which we took the electron and hole pockets to be spherically symmetric, but allowed the radii of the two pockets to vary. This model may be considered as a first approximation to the case of the Cr alloys, where by varying the electron-to-atom ratio, one may vary the size of the electron jack relative to that of the hole octahedron. This model correctly predicts the transition from a commensurate structure, when the sizes are equal, to an incommensurate structure, when the differences in the sizes becomes sufficiently great. However, the qualitative features in the limit $T_N \to 0$ predicted by this model are not in accord with experiment. The maximum in $\chi_0(\vec{Q})$ occurs at a regular maximum, whereas the experimental data are better fit by assuming a cusp-type maximum of form discussed in Sec. III. Clearly, a model band structure which combines these two features is necessary for the Cr alloys.

One important qualitative feature which the models do not reproduce is the first-order nature of the paramagnetic to antiferromagnetic transition. It is interesting to note that a small first-order transition similar to that found in Cr[21] has also been observed in Eu.[22] Of course, in the latter case the antiferromagnetism is not primarily itinerant in nature, but it is believed that the nesting of the conduction-electron Fermi surface plays an important role in the effective exchange and determines the period of the spin structure.

One mechanism which can cause a change in the order of a magnetic transition is the magnetostrictive effect proposed by Bean and Rodbell[23] for MnAs. Cohen *et al.*[20] have ruled out this mechanism in Eu, at least for simple distortions. In Cr, it is known that the antiferromagnetism is extremely sensitive to small volume changes. However, we have made estimates of the magnetostrictive effect in Cr and find that the coupling of the antiferromagnetism to the lattice is not strong enough to account for the first-order transition.

It is possible that strong-coupling corrections are important. One such correction is the change in effective interaction due to the loss of carriers in the AF phase. This was investigated for the Fedders-Martin model by Baklanov and Chaplik[24] who found no qualitative changes.

Note added in proof. Professor E. P. Wohlfarth has drawn the author's attention to the apparent inconsistency of the linear temperature dependence of $\chi_0(T)$ found in Sec. III with the thermodynamic requirement that the entropy vanishes in the limit $T \to 0$. The entropy S of a system of noninteracting electrons moving in a periodic potential and a magnetic field H_Q is given by the usual relation $S = \frac{1}{3}\pi^2 \times N(E_F)T$, where $N(E_F)$ is the density of states at the Fermi surface. It is straightforward to show that, for $Q = Q_0$, the wave vector of the Kohn cusp anomaly, $N(E_F)$ decreases initially linearly in $|H_Q|$. Thus for this Q vector there is a breakdown of analyticity and of the expansion of the free energy terms of H_Q^2 and T^2. This nonanalyticity is also apparent in the anomalous behavior of Δ and T_N discussed in the text. The author would like to thank Professor Wohlfarth for drawing his attention to this point.

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Study of the Spin-Reordering Transition in Cr_5S_6 †

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It is known that Cr_5S_6 becomes ferrimagnetic at $T_C = 305\,°K$ and undergoes a ferrimagnetic-antiferromagnetic transition at $150 < T_t < 160\,°K$. A neutron-diffraction study by van Laar indicates this transition to be of second order, whereas the existence of thermal hysteresis points to a first-order effect. We have investigated the magnetization of Cr_5S_6 as a function of hydrostatic pressure as well as of temperature and applied field. We find that $\partial T_C/\partial P = 1.83\,°K/kbar$, $\partial T_t/\partial P = 0.04\,°K/kbar$, and $\sigma_0^{-1}(\partial\sigma_0/\partial P) = -0.011/kbar$. $\partial T_t/\partial H$ runs from $-0.54\,°K/kOe$ at low fields to $-0.45\,°K/kOe$ at 9–12 kOe; these values, together with the shape of the normalized curve of magnetization versus temperature, are independent of pressure. In addition, we have investigated theoretically the classical ground-state spin configuration of the Cr_5S_6 lattice, using the generalized Luttinger-Tisza method, and have computed the thermal evolution of the ground state in the molecular field approximation. The observed spiral ground state is found to require not only that all the nearest-neighbor interactions be antiferromagnetic, but also that antiferromagnetic next-nearest-neighbor interactions be present. The calculated temperature dependencies of spins on the different sublattices lead directly to a second-order spin transition to a collinear ferrimagnetic configuration at T_t, in good agreement with experiment. We conclude that the transition at T_t is basically of second order, with secondary magnetostrictive forces responsible for the thermal hysteresis. The pressure dependence of σ_0 indicates that some of the magnetization of Cr_5S_6 arises from band electrons. The decrease of T_C with pressure is largely due to a decrease in the nearest-neighbor interaction along the c axis, which interaction is also the one most likely to involve band electrons.

I. INTRODUCTION

The structure of Cr_5S_6 has been determined as similar to that of NiAs, but with ordered vacancies.[1] The material is metallic,[2] has a ferrimagnetic Curie point of 305 °K, and undergoes a ferri-antiferromagnetic transition at 150–160 °K.[3–5] A recent neutron-diffraction study of Cr_5S_6 by van Laar[6] has shown the spin configuration to change from collinear Néel-type ferrimagnetism above the transition temperature (T_t) to a spiral configuration below T_t. van Laar also observed that the wave vector $\vec{k}$ which characterizes the spiral configuration varies in a smooth and continuous fashion from temperatures well below the transition to zero wavelength at and above T_t. This result indicates that the transition between the two magnetic states is of second order, but is at variance with the significant hysteresis observed for T_t, depending on whether the transition is observed during a heating or cooling cycle, which indicates a first-order transition.

In order to gain greater insight into the magnetic behavior of Cr_5S_6 we have undertaken a further study of its magnetic properties as functions of pressure as well as of magnetic field and temperature. We have also applied the generalized Luttinger-Tisza method[7] to study the ground-state configuration of Cr_5S_6 in a multidimensional magnetic-interaction parameter space. This has enabled us to establish the existence of a region in the space wherein the ground-state configurations are of the type observed by neutron diffraction. The variation with temperature of the configurations within this region was then studied in the molecular field approximation.

The effects of pressure on a sample of the slightly different material $CrS_{1.17}$ have been studied previously by Kamigaichi *et al.*[8] They noted kinks in the electrical conductivity at both T_t and T_C, and measured the changes in the temperatures of these kinks as functions of pressure. Since the measurements were of electrical conductivity, they could provide no insight to possible changes of a magnetic character. It also seemed preferable to choose a sample composition which more closely approximated the pure ferrimagnetic phase Cr_5S_6. As will be noted in Sec. II, our results at the transition temperature significantly differ from the results of Kamigaichi *et al.*[8]

II. EXPERIMENTAL RESULTS

Our measurements were made on a sample of