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Effect of spin fluctuations on the Stoner transition temperature*

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The low-frequency long-wavelength spin fluctuation modes make a major contribution to the free energy near the ferromagnetic instability of an itinerant-electron model. These fluctuations renormalize the static spin susceptibility and depress the transition temperature predicted by Stoner theory. Moriya and Kawabata (MK) have suggested a simple way of computing the depression self-consistently, by making sure the spin fluctuations go soft at the renormalized temperature T_c rather than at the Stoner value. We extend the discussion of MK to include both longitudinal and transverse spin fluctuations, and find a T_c which is only slightly smaller than T_c^{MK}. We also discuss the relation between T_c determined from the condition that the paramagnons go soft and that obtained by considering the softening of the spin waves. We argue that our new results give evidence that the basic MK procedure is internally consistent and somewhat less *ad hoc* than it appeared in its original presentation.

I. INTRODUCTION

Much of our current understanding of the magnetic properties of transition metals and their alloys is based on the so-called Stoner model.[1] This involves treating the exchange interaction between the d-band electrons in the mean-field approximation (MFA). Over the years, there have been many attempts[2] to improve upon the Stoner model of itinerant ferromagnetism. In particular, several recent theories[3-9] have tried to go past the MFA by including, in one way or another, the effect of spin fluctuations around the mean field. These fluctuation theories are attractive in that they make a definite improvement on the Stoner picture but still share with it a simple physical interpretation. We believe that of these self-consistent fluctuation theories, the simplest is that of Moriya and Kawabata (MK).[4,5]

In the present paper, we use the MK approach to determine the ferromagnetic transition temperature T_c. However, our analysis is an improved version since (a) it is based on a rotationally invariant form which involves both longitudinal and transverse spin fluctuations; (b) we show that the results are quite insensitive to the wave-vector cutoff q_c used as long as $q_c \lesssim 0.5 q_F$; and (c) we determine T_c self-consistently from the ferromagnetic phase side as well as from the paramagnetic phase side. More generally, we try to give some physical insight into the approximations involved in the MK approach. We feel that the results we have obtained show that the MK approach is internally consistent and somewhat less arbitrary than one might gather from a cursory examination of the original formulation. We might add, in this regard, that Kawabata[8] has recently shown how one may obtain something quite similar to the renormalized random-phase-approximation (RPA) results of MK using a graph-theoretic approach.

In Sec. II, we give a brief review of MK-I using a rotational invariant form of the interaction between the spins. We determine T_c^+ defined as the temperature at which the paramagnon modes go soft in Sec. III. In Sec. IV we discuss the renormalized spin-wave spectrum and determine T_c^-, the temperature at which the stiffness constant D vanishes. Section V is devoted to the relation between the classical fluctuation theory of Murata and Doniach[3,9] and the MK theory, both above and below T_c. Finally, we summarize our principal findings in Sec. VI and briefly comment on some recent theoretical work[6-9] which is relevant to the correctness of the MK method.

Throughout this paper we set $\hbar = 1$.

II. SELF-CONSISTENT THEORY OF THE SPIN-FLUCTUATION FREE ENERGY (PARAMAGNETIC PHASE)

We shall assume that the magnetic properties of the d-band electrons can be described by the rotational invariant Hamiltonian

$$\hat{H} = \sum_{\vec{k},\sigma} \epsilon_k \hat{a}^\dagger_{k\sigma} \hat{a}_{k\sigma} + \tfrac{1}{4} I_0 \hat{N} + \frac{1}{2} \sum_{\vec{q}} I_0 [\tfrac{1}{4} \hat{n}(\vec{q}) \hat{n}(-\vec{q}) - \vec{s}(\vec{q}) \cdot \vec{s}(-\vec{q})]. \quad (2.1)$$

Here $n(\vec{r})$ is the number operator for electrons at point $\vec{r}$, $\vec{s}(\vec{r})$ is the electronic spin-density operator, and I_0 is the intra-atomic exchange matrix element. We refer to Appendix A for more details on how one derives (2.1) starting with a system of d electrons interacting via a screened Coulomb interaction. As we discuss there, the interaction part of (2.1) is completely equivalent to the Hubbard Hamiltonian

$$\hat{V} = I_0 \sum_{\vec{q}} n_\uparrow(\vec{q}) n_\downarrow(-\vec{q}). \quad (2.2)$$

MK base their discussion on this form. The interaction (2.2) can be written in several different (but equivalent) ways involving spin-density operators. In particular, one has the transverse spin representation

$$\hat{V}^t = \tfrac{1}{2} I_0 \hat{N} - \tfrac{1}{2} I_0 \sum_{\vec{q}} [\hat{s}^+(\vec{q})\hat{s}^-(-\vec{q}) + \hat{s}^-(\vec{q})\hat{s}^+(-\vec{q})] \quad (2.3)$$

and the longitudinal reprentation

$$\hat{V}^l = I_0 \sum_{\vec{q}} [\tfrac{1}{4}\hat{n}(\vec{q})\hat{n}(-\vec{q}) - \hat{s}^z(\vec{q})\hat{s}^z(-\vec{q})]. \quad (2.4)$$

Moriya and Kawabata use (2.3) in their analysis, while we shall use (2.1). We note that the interaction term in (2.1) is equal to $\frac{1}{2}(\hat{V}^t + \hat{V}^l)$.

Let us assume we know the free energy $F(M)$ of our system described by (2.1) for a *given* value of the magnetization

$$M = \mu_0 \int d\vec{r}\, [n_\uparrow(\vec{r}) - n_\downarrow(\vec{r})], \quad (2.5)$$

where μ_0 is the magnetic moment of the electrons. Then the static spin susceptibility is given by the exact formula

$$\chi \equiv \frac{\partial^2 F(M)}{\partial M^2}\bigg|^{-1}_{M=\bar{M}}. \quad (2.6)$$

Here, M is set equal to its equilibrium value $\bar{M}$ at the end of the calculation. Following MK, it is convenient to write the total free energy in the form

$$F(M) = F_0(M) + F_{\mathrm{HF}}(M) + \Delta F(M). \quad (2.7)$$

Here $F_0(M)$ is the free energy in the absence of interactions and $F_{\mathrm{HF}}(M)$ is the Hartree-Fock part. These two give rise to the usual Stoner MFA results for χ. $\Delta F(M)$ includes all terms explicitly of order I^2 and higher, and will be referred to as the spin-fluctuation part. With this decomposition the paramagnetic spin susceptibility (2.6) is given by

$$\chi = 2\mu_0^2 N(T)/[1 - I_0 N(T) + \Lambda(I, T)], \quad (2.8)$$

where

$$N(T) \equiv -\int_{-\infty}^{\infty} d\epsilon\, N(\epsilon) \frac{df_0(\epsilon)}{d\epsilon} \quad (2.9)$$

and

$$\Lambda(I, T) \equiv 2\mu_0^2 N(T) \frac{\partial^2 \Delta F(M)}{\partial M^2}\bigg|_{M=0}. \quad (2.10)$$

$N(\epsilon)$ is the density of states per spin and $f_0(\epsilon)$ is the Fermi-Dirac distribution. By definition, the ferromagnetic transition temperature T_c^* is the solution of the equation

$$1 - I_0 N(T_c) + \Lambda(I, T_c) = 0, \quad (2.11)$$

since χ diverges when the temperature is decreased to this value. The Stoner MFA transition temperature, by way of contrast, is given by

$$1 - I_0 N(T_c^s) = 0. \quad (2.12)$$

We note that in the absence of spin fluctuations, the transition temperature is completely determined by the thermal distribution of electrons, i.e., $N(T)$.

By using a coupling constant integration[1] together with (2.1), we find that

$$\begin{aligned}\Delta F(M) = &\tfrac{1}{8} k_B T \sum_{\vec{q}, \omega_n} I_0 \int_0^1 d\lambda\, \chi^\lambda_{nn}(\vec{q}, i\omega_n; M) \\ &- \tfrac{1}{2} k_B T \sum_{\vec{q}, \omega_n} I_0 \int_0^1 d\lambda\, \chi^\lambda_{zz}(\vec{q}, i\omega_n; M) \\ &- \tfrac{1}{2} k_B T \sum_{\vec{q}, \omega_n} I_0 \int_0^1 d\lambda\, \Delta\chi^\lambda_{+-}(\vec{q}, i\omega_n; M),\end{aligned} \quad (2.13)$$

where

$$\Delta\chi^\lambda_{+-}(q, i\omega_n; M) \equiv \chi^\lambda_{+-}(q, i\omega_n; M) - \chi^0_{+-}(q, i\omega_n; M). \quad (2.14)$$

Here $\chi^\lambda_{+-}(M)$ and $\chi^\lambda_{zz}(M)$ are the usual dynamic transverse and longitudinal spin response functions for a system with a given total magnetization M and an exchange interaction of strength λI_0. We have subtracted χ^0_{+-} from the transverse part to ensure that $\Delta F(M)$ only contains terms of order I^2 and higher. Since (2.3) was used, the expression for $\Delta F(M)$ used in MK is simply twice the last term in (2.13). In (2.13), we sum over the Bose Matsubara frequencies $\omega_n = 2n\pi k_B T$, $n = 0, \pm 1, \pm 2, \ldots$.

In order to evaluate $\Delta F(M)$ using (2.13), we need to find the various response functions for a a given value of the magnetization M. These are well known in the RPA,[1,10,11] namely,

$$\chi^\lambda_{+-}(\vec{q}, \omega; M) = \frac{\chi^0_{+-}(\vec{q}, \omega; M)}{1 - \lambda I_0 \chi^0_{+-}(\vec{q}, \omega; M)}, \quad (2.15)$$

$$\chi^\lambda_{zz}(\vec{q}, \omega; M) - \tfrac{1}{4}\chi^\lambda_{nn}(\vec{q}, \omega; M) = \frac{\lambda I_0 \chi^0_\uparrow(\vec{q}, \omega; M)\chi^0_\downarrow(\vec{q}, \omega; M)}{1 - \lambda^2 I_0^2 \chi^0_\uparrow(\vec{q}, \omega; M)\chi^0_\downarrow(\vec{q}, \omega; M)}, \quad (2.16)$$

where

$$\chi^0_{+-}(\vec{q}, \omega; M) \equiv -\sum_{\vec{k}} \frac{f_0(\epsilon_{\vec{k}+\vec{q},\uparrow}) - f_0(\epsilon_{\vec{k}\downarrow})}{\omega - (\epsilon_{\vec{k}\downarrow} - \epsilon_{\vec{k}+\vec{q},\uparrow})}, \quad (2.17)$$

$$\chi^0_\sigma(\vec{q}, \omega; M) \equiv -\sum_{\vec{k}} \frac{f_0(\epsilon_{\vec{k}+\vec{q}\,\sigma}) - f_0(\epsilon_{\vec{k}\sigma})}{\omega - (\epsilon_{\vec{k}\sigma} - \epsilon_{\vec{k}+\vec{q},\sigma})}. \qquad (2.18)$$

Here the quasiparticle energies are given by

$$\epsilon_{\vec{k}\sigma} \equiv \epsilon_{\vec{k}} - \sigma\mu_0 \bar{H}; \quad \sigma = +1(\uparrow\text{spin}), -1(\downarrow\text{spin}). \qquad (2.19)$$

The effective magnetic field $\bar{H}$ is a known function of the net magnetization through the implicit relation

$$M = \mu_0 \sum_{\vec{k}} [f_0(\epsilon_{\vec{k}\uparrow}) - f_0(\epsilon_{\vec{k}\downarrow})]. \qquad (2.20)$$

To lowest order in T/T_F, we have

$$M = \mu_0 \{2N(0)\mu_0 \bar{H} - [F_1 N(0)/\epsilon_F^2](\mu_0 \bar{H})^3 + O((\mu_0 \bar{H})^5)\}, \qquad (2.21)$$

where $N(0)$ is the electronic density of states per spin at the Fermi level and F_1 is defined in Appendix B. We shall have use for (2.21) later.

We note $\epsilon_{\vec{k}\sigma}$ in (2.17) and (2.18) are functions of the given value of M but independent of the coupling strength λ. Using these RPA expressions in (2.13), the coupling constant integration can be done to give

$$\Delta F_{\text{RPA}}(M) = \frac{k_B T}{4} \sum_{\vec{q}, \omega_n} \ln[1 - I_0^2 \chi^0_\uparrow(\vec{q}, i\omega_n) \chi^0_\downarrow(\vec{q}, i\omega_n)] + \frac{k_B T}{2} \sum_{\vec{q}, \omega_n} \{\ln[1 - I_0 \chi^0_{+-}(\vec{q}, i\omega_n)] + I_0 \chi^0_{+-}(q, \omega_n)\}. \qquad (2.22)$$

Essentially the same result has been obtained[11,12] by summing up ring (longitudinal part) and ladder (transverse part) free-energy diagrams. We might note that (2.22) may be written in a more physically transparent form. This makes use of the fact that for any function $A(\omega)$ which is analytic off the real ω axis (as well as nonsingular at $\omega = 0$), we have

$$k_B T \sum_{\omega_n} A(i\omega_n) = \frac{1}{2} \int_c \frac{d\omega}{2\pi i} \coth(\omega/2k_B T) A(\omega) = -\int_c \frac{d\omega}{2\pi i} F_0(\omega) \frac{\partial A(\omega)}{\partial \omega}. \qquad (2.23)$$

Here the contour c encircles the positive and negative frequency axes in a counterclockwise sense but excludes the origin, while

$$F_0(\omega) = \tfrac{1}{2}\omega + k_B T \ln(1 - e^{-\omega/k_B T}) \qquad (2.24)$$

is the Helmholtz free energy of a boson excitation of energy ω. Using the second form in (2.23), we easily verify that ΔF_{RPA} in (2.22) may be reduced to

$$\Delta F_{\text{RPA}}(M) = \sum_i [F_0(\omega_i) - F_0(\omega_i^0)], \qquad (2.25)$$

where ω_i (ω_i^0) are the poles of the longitudinal and trasnverse spin susceptibilities of the interacting (noninteracting) system. (See Thouless[13] for details.) Thus we see that (2.22) is simply the total free energy of a system of noninteracting boson excitations corresponding to spin and density fluctuations.

Inserting (2.22) into (2.10), and making use of (2.21), we find by a straightforward calculation that

$$\Lambda(I, T) = k_B T \sum_{\vec{q}, \omega_n} R(\vec{q}, i\omega_n; I) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} [2N_0(\omega) + 1] \sum_{\vec{q}} \text{Im}\, R(\vec{q}, \omega - i0^+; I) \qquad (2.26)$$

where

$$R(\vec{q}, \omega) \equiv -\frac{1}{\chi_p} \frac{I_0^2}{4} \left(\frac{1}{1 - I_0 \chi^0} + \frac{1}{1 + I_0 \chi^0}\right) \left[\chi^0 \frac{\partial^2 \chi^0_\uparrow(\bar{H})}{\partial \bar{H}^2} - \left(\frac{\partial \chi^0_\uparrow(\bar{H})}{\partial \bar{H}}\right)^2\right]_{\bar{H}=0} - \frac{1}{\chi_p} \frac{I_0^2}{2} \left[\chi^0 \frac{\partial^2 \chi^0_{+-}(\bar{H})}{\partial \bar{H}^2} \frac{1}{1 - I_0 \chi^0} + \left(\frac{\partial \chi^0_{+-}(\bar{H})}{\partial \bar{H}}\right)^2 \frac{1}{[1 - I_0 \chi^0]^2}\right]_{\bar{H}=0}. \qquad (2.27)$$

In expressions such as (2.26), the part proportional to the Bose factor $N_0(\omega)$ gives the contribution of thermally excited fluctuations. The temperature-independent part gives the zero-point contribution. The temperature dependence of χ^0_{+-} and χ^0_σ is very small compared to that introduced by $N_0(\omega)$. Assuming that $T \ll T_F$, these are evaluated at $T = 0\,°\text{K}$. Finally, let us note that in deriving (2.27), use has been made of the relation

$$\left.\frac{\partial \chi^0_\uparrow}{\partial \bar{H}}\right|_{\bar{H}=0} = -\left.\frac{\partial \chi^0_\downarrow}{\partial \bar{H}}\right|_{\bar{H}=0}. \qquad (2.28)$$

Béal-Monod, Ma, and Fredkin[12] were the first to use (2.26) and (2.27) in order to evaluate the low-temperature spin susceptibility of an exchange-enhanced Fermi liquid. The low-frequency modes are expected to be the major contribution to $\Lambda(I, T)$ for two reasons. First of all, the factor coth(ω/

$2k_BT$) in (2.26) means that mode of energy $\omega \lesssim k_BT$ will be heavily weighted. Secondly, the function $\mathrm{Im}\, R(\vec{q}, \omega)$ itself develops a peak at the so-called paramagnon energy $\overline{\omega}$, given by

$$1 - I_0\chi^0(\vec{q}, \overline{\omega}) = 0. \qquad (2.29)$$

Using the well-known paramagnon expansion of $\chi^0(\vec{q}, \omega)$ for $\omega \ll \epsilon_F$ and $q \ll q_F$ [see Appendix B], the dispersion relation (2.29) reduces to

$$\overline{\omega} \simeq -ic_P q, \qquad (2.30)$$

with

$$c_P = \frac{v_F}{2A_1}\frac{1-\overline{I}}{\overline{I}}, \qquad (2.31)$$

where $\overline{I} \equiv I_0 N(T)$. One finds that the closer the system gets to the Stoner ferromagnetic instability, the intensity of the paramagnon peak in $\mathrm{Im}\, R(\vec{q}, \omega)$ increases while its frequency decreases. As a result, the low-frequency spin fluctuations make the increasingly dominant contribution to $\mathrm{Im}\, R(\vec{q}, \omega)$ the closer $\overline{I}$ is to unity.[1] In this regard, we might also emphasize that the RPA result (2.22) for ΔF is *only* expected to be a reasonable approximation for the free energy of long-wavelength, low-frequency modes. Fortunately, it is precisely the low-q/q_F, low-ω/ϵ_F region which is the important part when one is working with a system with strong exchange enhancement.

As MK point out, it is not consistent to evaluate $\Lambda(I, T)$ using (2.26) and then to use the result in (2.10) to determine the renormalized ferromagnetic transition temperature T_c. The reason is that the dominant contribution to $\Lambda(I, T)$ should come from spin fluctuations which go soft at T_c. When we use the RPA expression (2.27), the paramagnons go soft (i.e., $c_P \to 0$) at the Stoner temperature T_c^s, rather than at T_c. Following MK, the simplest self-consistent way of modifying (2.27) in order to remedy this is to make the change

$$\frac{1}{1 - I_0\chi^0(q, \omega)} \to \frac{1}{1 - I_0\chi^0(q, \omega) + \Lambda(I, T)}\,. \qquad (2.32)$$

This ensures that the important long-wavelength, low-frequency paramagnon modes go soft at T_c, since the renormalized paramagnon velocity is now given by

$$\tilde{c}_P = \frac{v_F}{2A_1}\frac{1-\overline{I}(T)+\Lambda(I,T)}{\overline{I}(T)}$$
$$\equiv \frac{v_F}{2A_1}\,\delta(I, T), \qquad (2.33)$$

in place of (2.31). With this renormalized version of $\tilde{R}(\vec{q}, \omega)$, we see that (2.26) now becomes a self-consistent equation for $\tilde{\Lambda}(I_0, T)$. [We sometimes use a tilde to represent the renormalized quantities based on using (2.32).]

As we noted in (2.25), ΔF in (2.22) is the free energy of the noninteracting spin-fluctuation modes. It seems reasonable, therefore, to require that these modes (which are the soft modes driving the transition) be defined relative to the new phase which they themselves help to produce. The ansatz (2.32) is equivalent to the assumption that as far as the important long-wavelength paramagnons go, they have the same structure as in the RPA, but go soft at the correct temperature. In this regard, it is clear that our use of (2.32) in (2.27) only makes sense because the paramagnon modes give the dominant contribution to $\Lambda(I, T)$. This is certainly the case for temperatures close to T_c but has less validity elsewhere.

Since (2.27) (and hence the MK self-consistent version of it) is at best only valid as a description of the long-wavelength modes, a $\vec{q}$-sum cutoff q_c must be introduced in (2.26). Numerical calculations we have performed show that as long as $q_c \lesssim 0.5q_F$, the results for $\tilde{\Lambda}(I, T)$ using (3.1) are insensitive to the value used for q_c. On the other hand, if we take $q_c > q_F$, as MK do, we find that not only is $\tilde{\Lambda}(I, T)$ quite cutoff-dependent, but a significant temperature-independent contribution to $\tilde{\Lambda}$ arises from fluctuations of high frequency ($\omega \gtrsim \epsilon_F$). In Table I, we show the values of the temperature-independent part of $\tilde{\Lambda}$ for different cutoffs. [In these calculations, we evaluated $\tilde{R}_t$ as given by (3.1) using a simple parabolic-band density of states.]

In summary, we feel it is only consistent to use the MK theory for modes $q \lesssim 0.5q_F$. There seems to be little basis in treating the shorter-wavelength spin fluctuations by anything as simple as the Moriya-Kawabata approach. Indeed, one might expect that for $q > q_c$, the unrenormalized RPA theory would be a better starting point. Of course, the temperature-independent part of Λ can be expected to be dominated by the short-wavelength spin fluctuations, which in turn are probably very band-structure dependent. In MK-II and succeeding papers by Moriya and coworkers, $\Lambda(T=0)$ (this is denoted by λ_0) is neglected on the grounds that only weak ferromagnets are being considered. Actually there is some reason to hope that a good estimate

TABLE I. Temperature-independent part of $\tilde{\Lambda} \equiv \Lambda_0^{(1)}\overline{I} + \Lambda_0^{(2)}$ for different cutoffs.

q_c/q_F	$\Lambda_0^{(1)}$	$\Lambda_0^{(2)}$
$1.20 \simeq 2^{1/3}$	0.055	0.551
1.0	0.005	0.358
0.5	−0.012	0.094
0.1	−0.0005	0.004

of $\Lambda(T=0)$ is now possible even for strong ferromagnets like Ni and Fe. We refer to the fact that in such systems, the short-wavelength spin-wave energies as determined by neutron scattering at $T \ll T_c$ can be explained quantitatively[14] using a standard RPA theory in conjunction with a realistic band structure. It would seem possible to use the same model to calculate $\Lambda(T=0)$ quite realistically. However, in the rest of this paper, we shall concentrate on the temperature-dependent part of $\Lambda(T)$ and effectively set $\Lambda(T=0)=0$. The resulting theory is still expected to be a considerable improvement over the original Stoner theory for any ferromagnet in which $T_c \ll T_F$.

III. CALCULATION OF THE TRANSITION TEMPERATURE FROM THE PARAMAGNETIC SIDE

Using the self-consistent spin-fluctuation theory discussed in Sec. II, we see that at T_c^+ as defined by (2.11), (2.27) may be approximated by

$$\tilde{R}(\vec{q},\omega) = -\frac{1}{2\mu_0^2 N(0)}\frac{I_0}{4}\frac{1}{N(0)-\chi^0}\left[\chi^0\chi_\uparrow^{0''} - (\chi^{0'})^2\right]_{\bar{H}=0} - \frac{1}{2\mu_0^2 N(0)}\frac{1}{2}\left[I_0\frac{\chi^0\chi_{+-}^{0''}}{N(0)-\chi^0} + \frac{(\chi_{+-}^{0'})^2}{[N(0)-\chi^0]^2}\right]_{\bar{H}=0}, \quad (3.1)$$

where the primes on the response functions indicate that we are taking their derivatives with respect to $\bar{H}$ and we note that $\chi^0(\vec{q}=0,\ \omega=0)=N(0)$. Calculation shows that the effect of the density fluctuations (zero sound) is very small and we have neglected it in writing down (3.1). In the important paramagnon regime, the leading-order terms are given by

$$\tilde{R}(q,\omega) = \tfrac{1}{2}[\tilde{R}_l(q,\omega) + \tilde{R}_t(q,\omega)], \quad (3.2)$$

where

$$\tilde{R}_l(q,\omega) \simeq \frac{\frac{1}{4}I_0(K_1+J_1^2)}{\epsilon_F^2[A_2(q/q_F)^2 + A_3(2\omega/qv_F)^2 - iA_1(2\omega/qv_F)]}, \quad (3.3)$$

$$\tilde{R}_t(q,\omega) \simeq \frac{\frac{1}{2}I_0 F_1}{\epsilon_F^2[A_2(q/q_F)^2 + A_3(2\omega/qv_F)^2 - iA_1(2\omega/qv_F)]} - \frac{\frac{1}{2}I_0 D_1^2(2\omega/qv_F)^2(q_F/q)^2}{\epsilon_F^2[A_2(q/q_F)^2 + A_3(2\omega/qv_F)^2 - iA_1(2\omega/qv_F)]^2}. \quad (3.4)$$

In contrast to all the other terms, the transverse contribution coming from the second term in the large square brackets in Eq. (3.1) is independent of I_0, which is somewhat unphysical. This is presumably a consequence of the fact that the numerators in the original RPA expression were not renormalized. MK have argued[5] that in fact this term should be multiplied by $\bar{I}$ (which is of order unity in the cases of interest). We have followed this procedure in writing down the last term in (3.4).

Making use of these results and integrating over q, we find (for $\omega \ll \epsilon_F$)

$$\sum_{q<q_c} \mathrm{Im}\,\tilde{R}(\vec{q},\omega) = \frac{3N}{4\epsilon_F}\frac{\pi\sqrt{3}}{18\epsilon_F}\left(\frac{A_1}{A_2}\right)^{1/3} \times\left(\frac{K_1+J_1^2}{2A_2} + \frac{F_1}{A_2} - \frac{2}{3}\frac{D_1^2}{A_1^2}\right)I_0\left(\frac{\omega}{\epsilon_F}\right)^{1/3} \equiv \frac{\bar{I}\Gamma}{\epsilon_F}\left(\frac{\omega}{\epsilon_F}\right)^{1/3}. \quad (3.5)$$

Using this in (2.26), we obtain[4]

$$\tilde{\Lambda}(I_0,T) = \Gamma\bar{I}\,[(2/\pi)\,\zeta(\tfrac{4}{3})\,\Gamma(\tfrac{4}{3})]\,(T/T_F)^{4/3} = 2.057\Gamma\bar{I}\,(T/T_F)^{4/3} \quad (3.6)$$

for the contribution due to thermally excited spin fluctuations, i.e., the part proportional to the Bose factor $N_0(\omega)$.

Inserting (3.6) into (2.11), T_c^+ is determined by the equation

$$1 - \bar{I}\,[1 - \tfrac{1}{12}\pi^2(T_c/T_F)^2 + \cdots] + \Lambda(T=0) + 2.057\Gamma\bar{I}\,(T_c/T_F)^{4/3} = 0, \quad (3.7)$$

where $\Lambda(T=0)$ denotes the contribution of the zero-point spin fluctuations. Neglecting this temperature-independent term, (3.7) gives

$$T_c^+/T_F = C[(\bar{I}-1)/\bar{I}]^{3/4};\quad C \equiv (2.057\Gamma)^{-3/4}. \quad (3.8)$$

Using numerical coefficients appropriate to a free electron gas (see Ref. 4 and Appendix B), we find

$$\Gamma = 2.87 + 2.38 \quad (3.9)$$

and hence $C=0.17$. In contrast, MK obtain $\Gamma = 2 \times 2.38$ and $C=0.18$. We feel that the fact that our symmetric treatment of longitudinal and transverse spin fluctuations is in such close agreement with the MK work based on the transverse spin representation is strong evidence that the MK way of introducing self-consistency is internally consistent. Moreover, it justifies working in the simpler transverse picture. In Fig. 1, we plot T_c/T_F vs $\bar{I}$ using (3.9) and compare it with the usual Stoner result which follows from (2.12),

$$T_c^s/T_F \simeq 1.103\,[(\bar{I}-1)/\bar{I}]^{1/2}. \quad (3.10)$$

On the same figure, we also show some numerical results which are based on using the full expression (3.1), for different values of the cutoff q_c. As

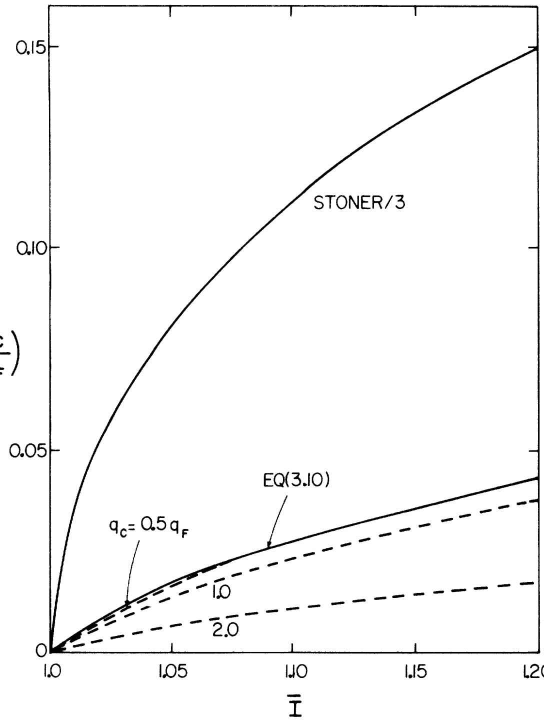

FIG. 1. T_c/T_F versus the Stoner parameter $\bar{I}$. Using several cutoffs, we also show the results based on the full expression (3.1). A single parabolic band has been used.

we mentioned at the end of Sec. II, the paramagnon regime dominates as long as $q_c \lesssim 0.5 q_F$ and the results are not very sensitive to the value of q_c. In this case, (3.5) is an excellent approximation for the result based on (3.1).

Let us emphasize that in *both* the Stoner and MK theories on which Fig. 1 is based, the condition for ferromagnetism is still $\bar{I}(T=0)>1$. This is because $\Lambda(T=0)$ has been neglected in (3.7). As MK argue, this is expected to be the case for weak ferromagnets; whether it can be safely omitted for an intermediate case like Ni is unknown at the present time. Still, the MK theory does enable us to say that even if the Stoner *criterion* for ferromagnetism at $T=0\,^\circ\mathrm{K}$ is even qualitatively correct, the Stoner theory still leads to a gross overestimate (roughly by a factor of 10) of the temperature at which ferromagnetism disappears. This is because T_c^s is determined by the number of noninteracting particle holes which are thermally excited around the Fermi surface while T_c^{MK} is determined by the number of low-frequency spin-fluctuation modes which are being thermally excited.

IV. FERROMAGNETIC REGION

Moriya and Kawabata have extended their approach to deal with the ferromagnetic phase[5] ($T<T_c$). In this section, we use their method to determine the ferromagnetic transition temperature T_c^-, defined as the temperature at which the propagating spin-wave modes go soft. We find that T_c^- and the T_c^+ obtained in Sec. III are essentially the same.

The analysis of the ferromagnetic regime[5] is based on the fact that the spontaneous magnetization $\bar{M}$ is determined by

$$\frac{\partial F(M,T)}{\partial M}\bigg|_{\bar{M}}=0=\frac{\partial F_0(M,T)}{\partial M}\bigg|_{\bar{M}}-\frac{I_0\bar{M}}{2\mu_0^2}+\frac{\partial \Delta F(M,T)}{\partial M}\bigg|_{\bar{M}}. \tag{4.1}$$

However, since we know that

$$\bar{H}(M,T)\equiv\frac{\partial F_0(M,T)}{\partial M}, \tag{4.2}$$

we can solve (4.1) for $\bar{M}(T)$ once we have decided on some appropriate approximation for the free energy $\Delta F(M,T)$. Within the RPA given by (2.22), we have

$$\frac{\partial \Delta F(M,T)}{\partial M}=k_BT\sum_{\vec{q},\omega_n}P(\vec{q},i\omega_n;M), \tag{4.3}$$

with

$$P(\vec{q},i\omega_n;M)\equiv-\frac{I_0^2}{4}\left[\left(\chi_\uparrow^0\frac{\partial\chi_\downarrow^0}{\partial M}+\chi_\downarrow^0\frac{\partial\chi_\uparrow^0}{\partial M}\right)\Big/\left[1-I_0^2\chi_\uparrow^0\chi_\downarrow^0\right]\right]-\frac{I_0^2}{2}\left(\chi_{+-}^0\frac{\partial\chi_{+-}^0}{\partial M}\Big/\left[1-I_0\chi_{+-}^0\right]\right). \tag{4.4}$$

The first term on the right-hand side comes from longitudinal fluctuations. In MK-II, $P(\vec{q},i\omega_n;M)$ is given by twice the second term (due to transverse spin fluctuations).

Since the fluctuation free energy $\Delta F(M,T)$ plays an important role [see (4.1)] in determining the value of $M(T)$ below T_c, we must base our discussion on a form of ΔF which gives the free energy of spin fluctuations whose dispersion relation is self-consistently determined. Following the argument of MK, the simple RPA expression in (4.4) can be made self-consistent by modifying the resonant denominators such that they vanish at the renormalized spin-fluctuation energies. However, the weights of these poles are not renormalized. Since we are only interested in temperatures just below T_c^-, where $\bar{M}(T)$ is very small, we need only concern ourselves with the low-frequency, long-wavelength spin-wave modes which go soft as $T\to T_c^-$. It is these modes which will make the dominant contribution to (4.3) as $T\to T_c^-$.

It is easy to verify that

$$\chi^0_{+-}(\vec{q}=0,\ \omega=0;M)=M/2\mu_0^2\bar{H}(M,T). \tag{4.5}$$

Clearly the second term on the right-hand side of (4.4) would not exhibit a spin-wave pole which went soft as $M\to 0$. However, if we make the transformation

$$\frac{1}{1-I_0\chi^0_{+-}(\vec{q},\omega;M)}\to\frac{1}{[I_0M/2\mu_0^2\bar{H}(M)]-I_0\chi^0_{+-}(\vec{q},\omega;M)}, \tag{4.6}$$

we see that the renormalized transverse part of (4.4) will exhibit low-frequency, long-wavelength spin-wave modes whose dispersion relation is given by (for a given value of M)

$$\mathrm{Re}\,\chi_{+-}(\vec{q},\omega;M)=M/2\mu_0^2\bar{H}(M). \tag{4.7}$$

Clearly this is consistent with the spin-wave modes going soft as $M\to 0$. For small values of q/q_F, the dispersion relation for a spin-wave mode in a cubic crystal is found to be

$$\omega=D(M)q^2, \tag{4.8}$$

with the stiffness coefficient given by the expression

$$D(M)=\frac{\mu_0}{6M}\sum_{\vec{q}}[f_0(\epsilon_{\vec{q}\uparrow})+f_0(\epsilon_{\vec{q}\downarrow})]\nabla^2_{\vec{q}}\epsilon_{\vec{q}} -\frac{1}{6\bar{H}M}\sum_{\vec{q}}[f_0(\epsilon_{\vec{q}\uparrow})-f_0(\epsilon_{\vec{q}\downarrow})](\nabla_{\vec{q}}\epsilon_{\vec{q}})^2, \tag{4.9}$$

with $\bar{H}\equiv\bar{H}(M)$ defined by (4.2). It is not hard to show that for any single band model, $D(M)$ in (4.9) is of order M when the magnetization is small. In particular, if we presume a parabolic band with some effective mass, then[15]

$$D(M)=\tfrac{1}{9}(M/\mu_0N)+O(M^3). \tag{4.10}$$

The poles of the longitudinal part of (4.4) do not correspond to the well-defined propagating spin-wave modes of the transverse part. However, they do exhibit fluctuations whose intensity becomes large in the limit as $M\to 0$ (somewhat reminiscent of paramagnons above T_c). We renormalize these modes in this limit, in a way analogous to our renormalization of the paramagnon modes in Sec. II.

We now have a way of computing the contribution of $\partial\Delta F(M,T)/\partial M$ due to long-wavelength transverse and longitudinal spin fluctuations whose dispersion relation depends on M. Using this in (4.1) we may then find the value of the magnetization $\bar{M}$ self-consistently and thus T_c^-. Working to lowest order in M and using (2.21), calculation shows that (4.4) in the paramagnon region is given by

$$\tilde{P}(\vec{q},\omega;M)=\tilde{R}(\vec{q},\omega)(M/\chi_p)+O(M^3), \tag{4.11}$$

where $\tilde{R}$ is given in (3.2) and $\chi_p\equiv 2\mu_0^2N(0)$. Thus we find

$$\frac{\partial\Delta\tilde{F}(M,T)}{\partial M}=\frac{\tilde{\Lambda}(I_0,T)}{\chi_p}M+O(M^3), \tag{4.12}$$

where $\tilde{\Lambda}(I_0,T)$ is defined in (3.6), and hence (4.1) reduces to

$$[1-I_0N(T)+\tilde{\Lambda}(I_0,T)]\bar{M}+O(\bar{M}^3)=0 \tag{4.13}$$

for T just below T_c^-. We have explicitly checked that the coefficient of the cubic term is positive and thus the transition is second order.

We see that as far as the longitudinal spin-fluctuation contributions are concerned, the MK approach of just renormalizing the RPA denominators leads to *identical* expressions for T_c^- and T_c^+. This is not so for the transverse contributions because of the anomalous term in (3.1) which is independent of I_0. However, the MK procedure of multiplying this term by $\bar{I}$ (~1) is indirectly justified[15] by the fact that the transverse contribution to T_c^+ then becomes identical to that obtained for T_c^-.

V. RELATION TO CLASSICAL FLUCTUATION THEORY

It can be argued that when a system is close to a second-order phase transition which is driven by soft modes, the dominant contribution to the free energy comes from the zero-frequency component ($\omega_n=0$).

Let us first consider the value of $\bar{M}$ just below T_c and work in the transverse representation (2.3). From the results of Sec. IV, we have the renormalized MK expression

$$\frac{\partial\Delta\tilde{F}(M)}{\partial M}=-k_BT\sum_{q<q_c'}\frac{I_0\chi^0_{+-}(\vec{q},M)\,\partial\chi^0_{+-}(\vec{q},M)/\partial M}{\chi^0_{+-}(0,M)-\chi^0_{+-}(\vec{q},M)}. \tag{5.1}$$

The cutoff q_c' is much less than q_c used earlier since it must incorporate the fact that only spin fluctuations of energy $\lesssim k_BT$ are to be included. Since q and M are small in the region of interest, we can use the expansion

$$\chi^0_{+-}(q,M)\equiv\chi^0_{+-}(q,\omega_n=0;M) =N(0)\left\{1-A_2\left(\frac{q}{q_F}\right)^2-\frac{1}{2}\left[F_1+F_3\left(\frac{q}{q_F}\right)^2\right]\times\left(\frac{\mu_0\bar{H}}{\epsilon_F}\right)^2+\cdots\right\}. \tag{5.2}$$

With this result, we can easily evaluate (5.1) to obtain (to lowest order in M)

$$\frac{\partial\Delta F(M,T)}{\partial M}=\frac{3N}{4\epsilon_F}\frac{I_0}{N(0)}\frac{k_BT}{\epsilon_F}\frac{F_1}{2A_2}\frac{M}{\mu_0^2}\frac{q_c'}{q_F}. \tag{5.3}$$

Using (5.3) and (2.21), (4.1) can be reduced to

$$\left(1-\bar{I}(T)+\bar{I}\,\frac{3N}{4\epsilon_F}\frac{1}{N(0)}\frac{T}{T_F}\frac{F_1}{A_2}\frac{q_c'}{q_F}\right)\bar{M}(T)=0. \quad (5.4)$$

In contrast with the results of Sec. IV, the fluctuation part in (5.4) is *very* dependent on the value of the cutoff q_c'. However (5.4) is equivalent to our preceding result (4.13) if we take the temperature-dependent cutoff to be

$$\frac{q_c'(T)}{q_F}=\frac{\tilde{\Lambda}(I_0,T)}{I_0}\frac{A_2}{F_1}\frac{T_F}{T}\frac{4\epsilon_F}{3N}\,. \quad (5.5)$$

In a simple parabolic-band model, $\tilde{\Lambda}(I_0,T)$ is given by (3.8) and thus (5.5) reduces to (see also Refs. 7 and 9)

$$\frac{q_c'(T)}{q_F}=11.11\,\frac{A_2}{F_1}\left(\frac{T}{T_F}\right)^{1/3}=2.78\left(\frac{T}{T_F}\right)^{1/3}\ll 1. \quad (5.6)$$

In the paramagnetic phase, as Moriya and Kawabata[5] have shown, keeping only the $\omega_n=0$ term leads to

$$\tilde{\Lambda}(I_0,T)=\frac{3N}{4\epsilon_F}I_0\frac{T}{T_F}\frac{F_1}{A_2}\frac{q_c'}{q_F}\left(1-\Pi^{1/2}\arctan\frac{1}{\Pi^{1/2}}\right), \quad (5.7)$$

where Π is essentially the inverse of the static spin susceptibility,

$$\Pi(T)\equiv\frac{q_F^2}{A_2q_c'^2}\,\delta(T)=\frac{\chi_P}{\chi}\frac{q_F^2}{A_2\bar{I}(T)q_c'^2}\,. \quad (5.8)$$

In deriving (5.7), we have made use of the fact that $q_c'\ll q_F$. Combining (2.8) with (5.7) and (5.8), the self-consistent equation for $\Pi(T)$ can be written in the form[5]

$$\Pi=-\frac{T_1}{T_0}+\frac{T}{T_0}\left(1-\Pi^{1/2}\arctan\frac{1}{\Pi^{1/2}}\right), \quad (5.9)$$

where

$$\frac{T_0}{T_F}\equiv\frac{A_2^2}{F_1}\frac{q_c'}{q_F}\left(\frac{3N}{4\epsilon_F}\frac{1}{N(0)}\right)^{-1}, \quad (5.10)$$

and

$$\frac{T_1}{T_F}\equiv\frac{\bar{I}-1}{\bar{I}}\frac{A_2}{F_1}\frac{q_F}{q_c'}\left(\frac{3N}{4\epsilon_F}\frac{1}{N(0)}\right)^{-1}. \quad (5.11)$$

Note that both T_0 and T_1 are dependent on T through q_c'. Clearly (5.9) has the solution $\Pi=0$ (i.e., $\chi\to\infty$) when $T=T_1(T)$. Thus (5.11) gives a value of T_c which is the same as that predicted by (5.4). Moreover, it is identical to our preceding results for T_c [see Secs. III and IV] if we choose the cutoff $q_c'(T)$ to be given by (5.5). We have also carried out similar calculations using a purely longitudinal representation (2.4) for the spin fluctuations. Without giving any details we simply state that Π is once more given by (5.9) close to T_c, the only change being the replacement

$$F_1\to\tfrac{1}{2}(K_1+J_1^2), \quad (5.12)$$

in the defining relations (5.10) and (5.11). For the electron gas, the relevant replacement is $\frac{1}{3}\to\frac{3}{8}$ (see Appendix B).

As pointed out by Moriya and Kawabata,[5] the $\omega_n=0$ approximation is especially interesting in that the results can be brought into contact with those derived by the quite different technique used by Murata and Doniach (MD).[3,9] Basically, the MD approach uses a functional-integral method to deal with the spin fluctuations. This approach yields a Ginzburg-Landau free energy F which includes quartic terms in the (longitudinal) magnetization, i.e.,

$$F=\int d\vec{r}\,\{a_1h^2(\vec{r})+a_2h^4(\vec{r})+a_3[\nabla h(\vec{r})]^2\}. \quad (5.13)$$

Fourier transforming and decoupling the quartic term in a mean-field approximation,[16] one has

$$F=k_BT\sum_{q<q_c'}\Omega(q)\,\bar{h}(\vec{q})\,\bar{h}(-\vec{q}), \quad (5.14)$$

where the "fluctuation energy" of mode q is $k_BT\Omega(q)$, with

$$\Omega(q)\equiv a_1+3a_2\langle\bar{h}^2\rangle+a_3q^2. \quad (5.15)$$

Here

$$\langle\bar{h}^2\rangle\equiv\sum_{q<q_c'}\langle\bar{h}(\vec{q})\,\bar{h}(-\vec{q})\rangle \quad (5.16)$$

and by explicit calculation of the thermal average using (5.14), one finds that

$$\langle\bar{h}^2\rangle=\sum_{q<q_c'}\frac{1}{\Omega(q)}\,. \quad (5.17)$$

In this model, the static spin susceptibility is given by

$$\chi=[2\mu_0^2(k_BT)^{-1}/\Omega(q=0)]. \quad (5.18)$$

Defining Π by

$$\Pi\equiv\frac{2\mu_0^2(k_BT)^{-1}}{\chi\,a_3q_c'^2}=\frac{a_1+3a_2\langle\bar{h}^2\rangle}{a_3q_c'^2}\,, \quad (5.19)$$

we see that (5.17) can be rewritten as

$$\langle\bar{h}^2\rangle=\frac{1}{a_3}\sum_{q<q_c'}\frac{1}{q^2+q_c'^2\Pi}\,. \quad (5.20)$$

The preceding two equations can be combined to find a self-consistent equation for Π,[3,16] namely,

$$\Pi=\frac{a_1}{a_3q_c'^2}+\frac{3}{2\pi^2}\frac{a_2}{a_3^2}\frac{1}{q_c'}\left(1-\Pi^{1/2}\arctan\frac{1}{\Pi^{1/2}}\right). \quad (5.21)$$

We observe that (5.21) has the same structure as (5.9). The Ginzburg-Landau parameters occurring in the MD theory are given by

$$a_1 = 1 - \bar{I},$$
$$a_2 = \tfrac{1}{6} K_1 \bar{I} (I_0/\epsilon_F)(T/T_F), \qquad (5.22)$$
$$a_3 = A_2 \bar{I},$$

for an itinerant model (these results are different from those in Refs. 3 and 9). The resulting transition temperature is given by

$$\frac{T_c^{\text{MD}}}{T_F} = \frac{\bar{I}-1}{\bar{I}} \frac{A_2}{K_1} \frac{q_F}{q_c'(T_c^{\text{MD}})} \left(\frac{3N}{4\epsilon_F} \frac{1}{N(0)} \right)^{-1}. \qquad (5.23)$$

Apart from the numerical coefficients, this result is identical to the result [see (5.11)] we obtained in the $\omega_n = 0$ approximation to the MK formalism. In particular, in the case of longitudinal fluctuations, the change is $K_1 \rightarrow \frac{1}{2}(K_1 + J_1^2)$. At least in the parabolic band approximation, these coefficients are comparable (see Appendix B) and thus the transition temperatures differ by very little.

Using functional-integral methods, several authors[6,9] have recently commented on the correctness of the original MD theory, i.e., to what extent (5.13) can be microscopically derived and also the validity of using a mean fluctuation-field approximation for the quartic term in (5.13). The main point we want to make here is that the MD result for the transition temperature is, in some sense, vindicated as a result of the quite different microscopic approach initiated by Moriya and Kawabata[4,5,8] which leads to a very similar result.

VI. CONCLUSION

Our major goal in this paper has been to give a detailed exposition of the MK theory of the ferromagnetic transition. In particular we have discussed several points which were not emphasized in the original work of MK, namely, (i) the theory only makes sense if the wave-vector cutoff q_c is somewhat less than q_F, (ii) equal weight is given to both the longitudinal and the transverse spin fluctuations, (iii) determination of T_c from both the paramagnetic and the ferromagnetic side, and (iv) emphasis on the MK theory as a soft-mode theory and the resulting relation to other discussions in the literature.

In assessing the MK theory as well as this paper, it is important to keep clearly in mind the fact that it is not an attempt at a rigorous theory of the ferromagnetic transition in metals. Rather it is an approach which generalizes the Stoner mean-field picture by including the effect of spin fluctuations in a simple, but still self-consistent, manner. Any value it has lies in its simplicity as well as the fact that it leads to an expression for T_c which involves, in an explicit manner, the long-wavelength low-frequency parts of the irreducible spin susceptibilities. For example, the constant C in (3.8) is given in terms of the band-structure-dependent constants K_1, J_1, F_1, A_1, and A_2 (see Appendix B). In this regard, future work on the MK theory might well be a systematic attempt at comparing its predictions for T_c with experimental data on transition metals and their alloys. It would be useful to extend the MK calculations to cover the case of alloys. We recall that the Stoner theory often has given some qualitative insight into how T_c varied with alloying and it would be of interest to see if the MK-type theory would make this more quantitative.

A more theoretical question is the precise relation between the MK theory and other more systematic attempts[6-9] to include fluctuations. Most of these are based on functional-integral methods and hence any direct comparison is difficult. However we have seen in Sec. V that the MK theory does give rise to very similar results as the MD calculation, which in turn may be viewed as a simple version of more systematic calculations.[6,9] We might also note that the MK theory, crude as it is, is not restricted to the static approximation.

A strength of the MK theory is that it is directly based on the free energy (2.25) of a system of uncoupled spin fluctuations, care being taken to renormalize the frequencies in a self-consistent manner. Thus while the way the renormalization is done is somewhat *ad hoc*, at least it involves a quantity (the spin-fluctuation frequency) which has a direct physical significance. This is to be contrasted with the situation in other methods.[6-9]

One problem in which one expects the inclusion of spin fluctuations to be important is in determining how the ferromagnetic transition temperature of thin metallic films depends on the thickness. A very detailed analysis based on the Stoner theory has been recently given.[17] We hope to extend that work to include spin fluctuations in a future publication using the MD method.

It is quite straightforward to apply the MK formalism (as well as the MD approach) to a 2-*d* electron gas. The results[18] are consistent with the expectation that such a system never exhibits a ferromagnetic phase. However we feel there is some question of how internally consistent such calculations are. We recall that the whole MK approach is built on the low-frequency spin fluctuations becoming dominant near T_c and making use of this fact to develop a simple theory of the effect of these fluctuations. This whole justification is removed when one is dealing with a system in which the spin fluctuations never go soft, i.e., χ is always finite. As we have stated earlier, while the whole MK approach makes sense very close to T_c, it breaks down when one is far from T_c or, more especially, when there is no transition. This criticism also applies to the recent calculation of Ramakrishnan[7] of the spin susceptibility of a 2-d model of nickel.

Finally, let us emphasize that while we feel the MK theory as discussed in this paper gives an adequate estimate of the effect of thermal fluctuations, nothing has been said about the temperature-independent part of Λ in (2.8), i.e., the zero-point energy of the short-wavelength spin fluctuations. However, we feel that the ferromagnetic *instability* will be determined by the excitation of low-frequency spin fluctuations as long as T_c is somewhat less than the Fermi temperature. This driving mechanism is different from that in the original Stoner theory for T_c and, in fact, leads to a transition temperature which is about 10 times smaller whatever the value of $\bar{I}(T=0)$ (see Fig. 1). As a starting point, we feel the MK theory should be used in place of the Stoner theory (even for intermediate ferromagnets) when one is estimating the transition temperature.

APPENDIX A

In this Appendix, we discuss the relation between (2.1) and the more fundamental interaction between d electrons. In the localized site representation, the latter is given by[19]

$$\hat{V}=\frac{1}{2}\sum_{\sigma,\sigma'}\sum_{\substack{i,j\\i',j'}} V_{iji'j'}\hat{a}^\dagger_{i\sigma}\hat{a}^\dagger_{j\sigma'}\hat{a}_{j'\sigma'}\hat{a}_{i'\sigma}, \tag{A1}$$

where $V_{iji'j'}$ is the matrix element of an appropriately screened Coulomb interaction. We shall only keep the one-site ($i=j=i'=j'$) and two-site ($i=i'$, $j=j'$; $i=j'$, $j=i'$) terms and use the notation

$$V_{ijij}\equiv K_{ij};\quad V_{ijji}\equiv I_{ij};\quad V_{iiii}\equiv I_0 . \tag{A2}$$

The single-site contribution to (A1) is

$$\hat{V}_1=\tfrac{1}{2}I_0\sum_{\sigma,\sigma'}\sum_i \hat{a}^\dagger_{i\sigma}\hat{a}^\dagger_{i\sigma'}\hat{a}_{i\sigma'}\hat{a}_{i\sigma}. \tag{A3}$$

Using the identities $\hat{a}^2_{i\sigma}=0$ and $\hat{n}^2_{i\sigma}=\hat{n}_{i\sigma}$, this can be expressed in the Hubbard form [which is equivalent to (2.2)]

$$\hat{V}_1=\tfrac{1}{2}I_0\sum_\sigma\sum_i \hat{n}_{i\sigma}\hat{n}_{i,-\sigma}, \tag{A4}$$

as well as in the alternative forms

$$\hat{V}_1=I_0\sum_i\left(\tfrac{1}{4}\hat{n}_i\hat{n}_i-\hat{s}^z_i\hat{s}^z_i\right) \tag{A5}$$

and

$$\hat{V}_1=\tfrac{1}{4}I_0\hat{N}+\tfrac{1}{2}I_0\sum_i\left(\tfrac{1}{4}\hat{n}_i\hat{n}_i-\vec{s}_i\cdot\vec{s}_i\right). \tag{A6}$$

Here we have introduced the usual spin operators

$$\hat{s}^+_i\equiv\hat{a}^\dagger_{i\uparrow}\hat{a}_{i\downarrow};\quad \hat{s}^-_i\equiv\hat{a}^\dagger_{i\downarrow}\hat{a}_{i\uparrow};\quad \hat{s}^z_i\equiv\tfrac{1}{2}(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow}). \tag{A7}$$

The two-site contribution to (A1) corresponds to interaction between different sites. After a little algebra, this can be written in the form

$$\hat{V}_2=\frac{1}{2}\sum_{\substack{i,j\\ \neq}}(K_{ij}-I_{ij})\hat{n}_i\hat{n}_j+\sum_{\substack{i,j\\ \neq}} I_{ij}\left(\tfrac{1}{4}\hat{n}_i\hat{n}_j-\vec{s}_i\cdot\vec{s}_j\right). \tag{A8}$$

The second sum on the right-hand side of (A8) is due to interatomic exchange and clearly has the same structure as the part arising from intra-atomic exchange [see (A6)]. It is a straightforward matter to extend the discussion in Sec. II of this paper so as to include the contribution of (A8) in addition to that of (A6).

As a final remark, we note that (A6) is manifestly rotational invariant in spin space and is the form on which most field-theoretic discussions are based.[11,12] However one can also rewrite the Hubbard Hamiltonian (A4) in the form

$$\hat{V}_1=\tfrac{1}{2}I_0\hat{N}-\tfrac{2}{3}I_0\sum_i\vec{s}_i\cdot\vec{s}_i \tag{A9}$$

and sometimes this rotationally invariant form has been advocated.[20] In an exact calculation, of course, all the different ways of expressing (A4) would lead to the same results. However, this is not true in approximate calculations and the question then is to decide which is best. We feel that (A6) is to be preferred since it includes both longitudinal and transverse fluctuations on an equal basis.

APPENDIX B

We give here the susceptibilities and their derivatives in the paramagnon limit ($\omega\ll\epsilon_F$, $q\ll q_F$, $2\omega/qv_F\ll 1$), for a single isotropic-band model:

$$\chi^0(\vec{q},\omega)=N(0)\left[1+iA_1 2\omega/qv_F-A_2(q/q_F)^2-A_3(2\omega/qv_F)^2+\cdots\right], \tag{B1}$$

$$\left.\frac{\partial\chi^0_{+-}(q,\omega)}{\partial\bar{H}}\right|_{\bar{H}=0}=\frac{\mu_0}{\epsilon_F}N(0)\left[D_1\frac{2\omega}{qv_F}\frac{q_F}{q}+D_2\frac{2\omega}{qv_F}\frac{q}{q_F}+\cdots\right], \tag{B2}$$

$$\left.\frac{\partial\chi^0_\sigma(q,\omega)}{\partial\bar{H}}\right|_{\bar{H}=0}=\sigma\frac{\mu_0}{\epsilon_F}N(0)\left[J_1+J_2\left(\frac{q}{q_F}\right)^2+J_3\left(\frac{2\omega}{qv_F}\right)^2+\cdots\right], \tag{B3}$$

$$\left.\frac{\partial^2\chi^0_{+-}(q,\omega)}{\partial \overline{H}^2}\right|_{\overline{H}=0} = -\frac{\mu_0^2}{\epsilon_F^2}N(0)\left[F_1+F_2\left(\frac{2\omega}{qv_F}\right)^2\left(\frac{q_F}{q}\right)^2 + F_3\left(\frac{q}{q_F}\right)^2+\cdots\right], \quad \text{(B4)}$$

$$\left.\frac{\partial^2\chi^0_{\sigma}(q,\omega)}{\partial \overline{H}^2}\right|_{\overline{H}=0} = -\frac{\mu_0^2}{\epsilon_F^2}N(0)\left[K_1+K_2\left(\frac{q}{q_F}\right)^2+K_3\left(\frac{2\omega}{qv_F}\right)^2+\cdots\right]. \quad \text{(B5)}$$

For a 3-d electron gas with a parabolic band, the numerical coefficients are (the transverse susceptibility results are in agreement with those given in Ref. 4)

$$A_1=\tfrac{1}{4}\pi,\ A_2=\tfrac{1}{12},$$
$$D_1=\tfrac{1}{2},\ F_1=\tfrac{1}{3},$$
$$J_1=\tfrac{1}{2},\ J_2=\tfrac{1}{24},\ J_3=\tfrac{1}{8}, \quad \text{(B6)}$$
$$K_1=\tfrac{1}{2},\ K_2=\tfrac{1}{12},\ K_3=\tfrac{1}{4}.$$

More generally, the coefficients can be worked out for a band structure which more closely simulates that of transition metals. For an isotropic band, every coefficient [with the exception of A_1 in (B1)] can be written[21] in terms of $N(0)$, $N'(0)$, and $N''(0)$, where $N'(0)$ and $N''(0)$ are the first and second derivatives with respect to energy of the density of states at the Fermi level.

For an arbitrary band structure, J_1, F_1, and K_1 are still fairly simple because they involve the $q \to 0$ limit. One finds

$$J_1=\frac{N'(0)}{N(0)}\epsilon_F,$$
$$F_1=\left[\left(\frac{N'(0)}{N(0)}\right)^2-\frac{N''(0)}{3N(0)}\right]\epsilon_F^2, \quad \text{(B7)}$$
$$K_1=\left[\left(\frac{N'(0)}{N(0)}\right)^2-\frac{N''(0)}{N(0)}\right]\epsilon_F^2.$$

In contrast, the coefficients A_1 and A_2 (which enter prominently into the expressions for T_c) are somewhat complex.[21,22]

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