Microscopic theory of spin fluctuations in itinerant-electron ferromagnets. I. Paramagnetic phase

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In microscopic theories of phase transitions occurring in itinerant-electron systems, physical phenomena are generally considered in the random-phase (RPA) or mean-particle-field approximation. We describe here a many-body theoretical method of calculating the appropriate order-parameter susceptibility function $\chi(q,\omega^+)$ which goes beyond the RPA. A diagrammatic analysis of the equation of motion for a quantity related to $\chi(q,\omega^+)$ is made, and it is shown how one can systematically and self-consistently include the effect of order-parameter fluctuations on $\chi(q,\omega^+)$. The method is applied here to the paramagnetic phase of an itinerant-electron ferromagnet. A mean-fluctuation-field approximation (MFFA) which includes the contribution of one internal spin fluctuation to $\chi(q,\omega^+)$ is discussed in detail. Its temperature-dependent contribution to χ^{-1} goes roughly as $(k_B T \rho_{\epsilon_F})^{4/3}$. A self-consistent solution of the MFFA equation for $\chi(0,0)$ leads to a Curie-Weiss-like behavior for it. We make an explicit comparison of our results with experimental values for Ni, and find good agreement in the range $0.1 \leq (T-T_c)/T_c = \epsilon \leq 0.6$. In the Stoner or RPA theory the Curie-Weiss law is ascribed to the T^2 part of the particle-field term $-U\int f^{-\prime}(E)\rho(E)\,dE$. This is smaller than the MFF term by a factor $(k_B T\rho_{\epsilon_F})^{-2/3}$, and for Ni, is only 5% of the latter. The Curie-Weiss-like law observed in metallic paramagnets is therefore due to the mean spin-fluctuation field, as also realized by Murata and Doniach, and by Moriya and Kawabata. Going beyond the MFFA, we calculate the contribution of the simplest spin-fluctuation correlation diagram. The contribution of this diverges logarithmically as $\epsilon \to 0$. When this term becomes comparable to the MFFA, we are well in the critical regime which cannot be conveniently discussed by this method. This criterion is used to provide a first-principles estimate of the static and dynamic critical regimes in Ni. The former obtains for $\epsilon \lesssim 0.05$ and the latter for $\epsilon \lesssim 0.06(q/k_F)$. We show how spin fluctuations suppress ferromagnetism in a two-dimensional system and plot $\chi_{2d}(0,0)$ vs T for a Ni-like film in the MFFA. The method developed here can be applied to discuss fluctuation effects in the ferromagnetic phase, in superconductivity, and in itinerant-electron antiferromagnetism.

I. INTRODUCTION

Microscopic theories of phase transitions in itinerant-electron systems generally use the random-phase (RPA) or mean-particle-field approximation (MPFA). Well-known examples are the Gor'kov-Anderson[1] theory of superconductivity, the Stoner[2] model for ferromagnetism, and the Fedders-Martin[3] model for antiferromagnetism. This approximation is most successful for superconductors, the physical reason being the large zero-temperature order-parameter coherence length ξ_0 (in tin, $\xi_0 = 2.3\times 10^3$ Å), which considerably reduces fluctuation effects. In a ferromagnet, however, the coherence length is small, of the order of atomic dimensions (~2 Å).[4,5] We thus expect magnetic fluctuations to affect significantly the properties of itinerant-electron ferromagnets. The same can be said of itinerant-electron antiferromagnetism. We present in this paper a many-body theoretical method of calculating the effect of order-parameter fluctuations on the dynamic (order-parameter) susceptibility $\chi(\vec{q}, z_m)$ using the example of itinerant-electron ferromagnetism. A mean-fluctuation-field approximation (MFFA) is described in which the average effect of spin fluctuations on $\chi(\vec{q}, z_m)$ is considered. This effect is shown to be significant over a wide temperature range, and to lead to the observed Curie-Weiss behavior[6-8] behavior above T_c. A first-principles estimate is also obtained of the critical regime, i.e., the temperature range around T_c where fluctuation interactions become important. The method is not suitable for determining critical behavior.[5,9] The work described here therefore connects the RPA or mean-particle-field theory results which are valid far away from T_c and the interacting classical magnetic-fluctuation-field results[9] which are valid very close to T_c. The middle ground is charted here for the paramagnetic phase ($T > T_c$). In a later paper, we will discuss corresponding results for the ferromagnetic phase.[10] In the remainder of Sec. I, we outline the method used and the results obtained.

We are interested in calculating the wave vector ($\vec{q}$) and frequency (z_m) dependent order-parameter susceptibility (correlation function). In the ferromagnetic case, this is the spin susceptibility function $\chi(\vec{q}), z_m) = \chi^t(\underline{q})$. This is well known to be related to a two-particle Green's function G^{II} [see Eq. (2.2)]. The equation of motion for G^{II} relates it to a three-particle Green's function G^{III} (see Sec. II). We make a diagrammatic spin-fluctuation analysis of $G^{III}(\underline{q})$ and hence of $\chi(\underline{q})$. This means the following. G^{III} can be written, in principle, as a sum of an infinite number of diagrams; these diagrams will involve as basic units the single-particle Green's function G and the two-particle spin-singlet and spin-triplet scattering amplitudes, Γ^s and Γ^t (Fig. 1). Since near the phase transition the static spin susceptibility or the long-wavelength, low-energy spin-triplet scattering amplitude Γ^t is large, we separate out from the diagrams for $G^{III}(\underline{q})$ those (coherent) parts which are proportional to $\Gamma^t(\underline{q})$ ($\underline{q}$ is the momentum energy transfer in the particle-hole channel 13). The diagrams left out form an incoherent remainder which does not strongly depend either on the temperature or on the interaction strength. We further analyze the coherent part. Retention of the term containing only one Γ^t leads to the RPA result. Since spin fluctuations are large and their amplitude depends strongly on temperature, one should investigate coherent diagrams which involve more Γ^t's [see, for example, Fig. 2(b)]. We examine in detail and evaluate diagrams for G^{III} [and thence for $\chi(\underline{q})$] which have *one* more Γ^t or spin fluctuation in addition to $\Gamma^t(\underline{q})$. If we also include such terms in the equation for $\chi(\underline{q})$, we have self consistently included the effect of the mean particle field (RPA), *and* the effect of one internal spin fluctuation on the spin susceptibility $\chi(\underline{q})$. This approximation is called the mean-fluctuation-field approximation (MFFA).

The spin susceptibility $\chi(\underline{q})$ is evaluated in the MFFA in Sec. III. It is found that the contribution of the fluctuation field to $\chi(0,0)^{-1}\chi_P$ is of the form $A+B(k_BT\rho_{\epsilon_F})^{4/3}$ (here χ_P is the Pauli susceptibility, A and B are constant, and B is positive; ρ_{ϵ_F} is the density of states at the Fermi energy). The RPA contribution is $+U\int f^{-\prime}(\epsilon)\rho(\epsilon)\,d\epsilon$ where U is the zero-range Coulomb repulsion between electrons. We see that spin fluctuations tend to suppress ferromagnetism. The contribution of the constant part (A term) can be included by suitably redefining the $T=0$ RPA term $-U\rho_{\epsilon_F}$, i.e., by changing U to U_{eff}. Since we are discussing here a degenerate electron gas, we have $k_BT\rho_{\epsilon_F}\ll 1$, and thus the temperature-dependent spin-fluctuation contribution is small in comparison to the RPA term which (with U_{eff} replacing U) gives the correct zero-order contribution $-U_{\text{eff}}\rho_{\epsilon_F}$. However, since in the vicinity of the phase transition, $\chi(0,0)^{-1}\chi_P\to 0$, the spin-fluctuation term contributes a very important correction, and indeed determines the temperature dependence of $\chi(0,0)^{-1}\chi_P$. We make a numerical calculation for Ni, and show that in a relatively wide temperature range, $0.1\lesssim k_BT\rho_{\epsilon_F}\lesssim 0.15$ ($k_BT_c\rho_{\epsilon_F}\simeq 0.090$) the observed susceptibility is well described in the MFFA (Fig. 3). We suggest, therefore, that the Curie-Weiss law observed for the temperature dependence of $\chi(0,0)$ in itinerant-electron ferromagnets above T_c is due to the presence of this spin-fluctuation term. In the Stoner model or RPA, the observed Curie-Weiss law is explained through the temperature dependence of the mean particle field, i.e., the temperature dependence of $-\int f_\epsilon^{-\prime}\rho(\epsilon)\,d\epsilon$. This is proportional to $(k_BT\rho_{\epsilon_F})^2$ and is thus, in principle, smaller than the spin-fluctuation term. In the case of Ni, calculation (Sec. III) shows this "Stoner" term to be only 5%

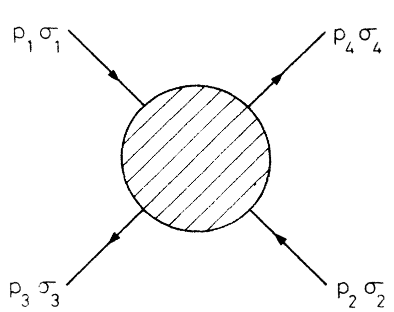

FIG. 1. The two-particle scattering amplitude $\Gamma(p_1\sigma_1, p_2\sigma_2, p_3\sigma_3, p_4\sigma_4)$ with energy momentum and spin indices labeled.

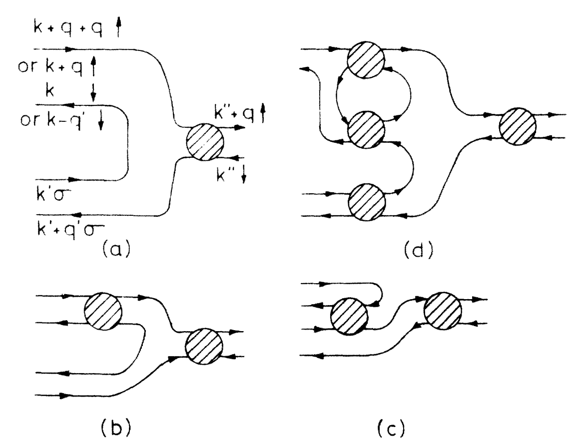

FIG. 2. Some coherent diagrams for $G_k^{III}(\underline{q})$ [see Eq. (2.4)]. As is evident from the definition, the diagrams consist, in general, of incoming electron-hole pairs ($\underline{k}+\underline{q}+\underline{q}'\uparrow$, $\underline{k}\downarrow$) (*or* $\underline{k}+\underline{q}\uparrow$, $\underline{k}-\underline{q}'\downarrow$) and ($\underline{k}'\sigma$, $\underline{k}'+\underline{q}'\sigma$), and an outgoing electron-hole pair ($\underline{k}''+\underline{q}\uparrow$, $\underline{k}''\downarrow$). The four-momenta $\underline{k}'$ and $\underline{k}''$ are summed over. Some examples are shown above. (a): an RPA diagram. Here the blob represents the spin-triplet scattering amplitude $\Gamma^t(\underline{q})$. (b) and (c): diagrams with one more Γ^t. These are among the one-spin-fluctuation terms [Eq. (2.13)]. (d): a three-spin-fluctuation term.

of the spin-fluctuation term. Thus the explanation of a Curie-Weiss law using the temperature dependence of the RPA contribution is *not* tenable, in view of the existence and magnitude of the temperature-dependent spin-fluctuation contribution to $\chi(0,0)$. Further qualitative differences between the predictions of RPA and the MFFA show up in the spin susceptibility of a two-dimensional itinerant-electron system. The RPA predicts a phase transition at an appropriate value of U_{eff}. In the MFFA, we find, in accord with general results, that the phase transition is suppressed by fluctuations. Furthermore, we can explicitly calculate $\chi_{2d}(T)$. We perform such a calculation for a film with the band parameters of Ni (see Fig. 3).

From the above it may appear that for three-dimensional systems an expansion for the temperature-dependent properties of G^{III} [or $\chi(\underline{q})$] in powers of the spin fluctuation is rapidly convergent, the expansion parameter being $(k_B T\rho_{\epsilon_F})^{4/3} \ll 1$. It is true that in general an nth-order diagram (i.e., one with n internal Γ^t's) contributes terms of order $(k_B T\rho_{\epsilon_F})^{4m/3}$ $(0 \leq m \leq n)$ relative to the RPA term. The $m=0$ term modifies the RPA condition, i.e., U is modified to U_{eff}. The $m=1$ term influences the coefficient of the one-spin-fluctuation term for the Curie-Weiss temperature dependence of χ. The terms with $m \geq 2$ can be neglected. There is however a class of diagrams (spin-fluctuation correlation diagrams) which

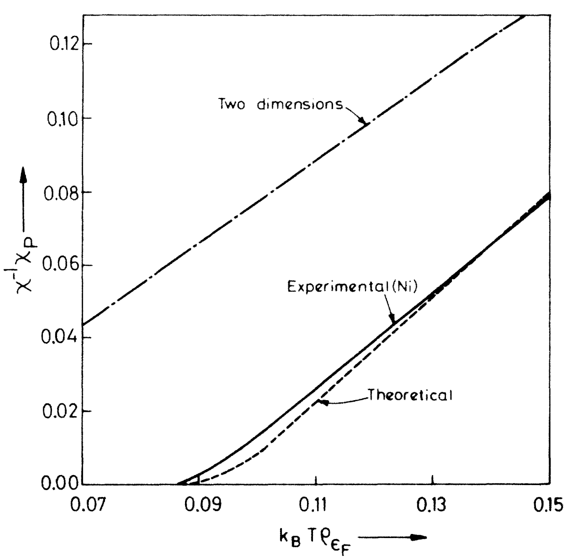

FIG. 3. The static inverse susceptibility χ^{-1} of Ni (times the Pauli value χ_P) plotted against temperature (times $k_B\rho\epsilon_F$). Solid line represents the experimental value, the value calculated in the MFFA being shown by the broken line. The calculated $\chi^{-1}(0,0)$ for a two-dimensional film with band parameters of bulk Ni is shown by the dot-dashed line.

contribute singularly as $T \rightarrow T_c$. Their contribution diverges as $\ln(T-T_c)$ or powers thereof. These diagrams, representing correlations between spin fluctuations, determine the critical behavior. The microscopic theory used in this paper is quite cumbersome and cannot be (easily) used to evaluate, for example, the critical indices.[5,9] We perform (Sec. IV) a calculation of the terms in G^{III} having four Γ^t's, one of them being $\Gamma^t(\underline{q})$ and the other three being internal spin fluctuations whose momentum and energy are integrated over. This represents the first significant fluctuation correlation correction to the MFFA. One is well in the critical regime when the contribution of the former is comparable to that of the latter for $\chi^{-1}\chi_P$. For nickel, it is found that the static critical regime sets in around $\epsilon=(T-T_c)/T_c \lesssim 0.05$ and the dynamical critical regime around $\epsilon = 0.06q$, where q is the wave vector in units of k_F.

The Curie-Weiss law for itinerant-electron ferromagnets has been obtained earlier by Murata and Doniach,[6] and by Moriya and Kawabata.[7] The former authors use a semiphenomenological Ginzburg-Landau functional for the itinerant-electron system, with magnetization as the order parameter. The latter authors use an RPA-like form for $\chi(\underline{q})$ and estimate the spin-fluctuation contribution to it by requiring consistency between two different ways of calculating $\chi(0,0)$. (See Sec. V for a more detailed description of these methods and for their comparison with the method and results of this paper). We present in this paper a fully microscopic and fairly general investigation of fluctuation effects. In the concluding section (Sec. V) we suggest that spin-fluctuation effects are important in nearly ferromagnetic Fermi systems and in ferromagnets below T_c.

II. FORMALISM AND THE MEAN-FLUCTUATION-FIELD APPROXIMATION

A. Formalism

The itinerant-electron system is described by the Hamiltonian

$$H=\sum_{\vec{k},\sigma} \epsilon_{\vec{k}} a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma} + \tfrac{1}{2} U \sum_{\vec{q}} \rho_{\vec{q}}\rho_{-\vec{q}} . \qquad (2.1)$$

The first term describes free electrons, the energy of an electron in the state $\vec{k}\sigma$ being $\epsilon_{\vec{k}}$; $a^\dagger_{\vec{k}\sigma}$, $a_{\vec{k}\sigma}$ are the creation and annihilation operators, respectively, for an electron in the state $\vec{k}\sigma$. The second term represents a zero-range repulsion between electrons, of magnitude U. $\rho_{\vec{q}}$ is the density-fluctuation operator, i.e., $\rho_{\vec{q}} = \sum_{\vec{k}\sigma} a^\dagger_{\vec{k}+\vec{q}\sigma} \times a_{\vec{k}\sigma}$. We are interested in evaluating the dynamic spin susceptibility $\chi(\underline{q})$. In the paramagnetic phase, the system is rotationally invariant; therefore longitudinal and transverse susceptibilities are the same. It is more convenient to evaluate the transverse susceptibility, which is given by the Kubo formula[11]

$$\chi(\vec{q}, z_m) = 2\mu_B^2 \chi(\underline{q}) = 2\mu_B^2 \int_0^\beta \langle T\{S_{\vec{q}}^+(v) S_{-\vec{q}}^-(0)\}\rangle e^{-vz_m} dv . \quad (2.2)$$

Here μ_B is the Bohr magneton and $z_m = 2mi\pi/\beta$, m being an integer. The spin-fluctuation creation operator $S_{\vec{q}}^+ = a^\dagger_{\vec{k}+\vec{q}\uparrow} a_{\vec{k}\downarrow}$ and $S_{-\vec{q}}^-$ is its Hermitian adjoint. The operator $S_{\vec{q}}^+$ can be written as $S_{\vec{q}}^+ = \sum_{\vec{k}} S^+_{\vec{k},\vec{q}}$, where $S^+_{\vec{k},\vec{q}} = a^\dagger_{\vec{k}+\vec{q}\uparrow} a_{\vec{k}\downarrow}$. Similarly, one can write

$$\chi^t(\underline{q}) = \sum_{\vec{k}} \int_0^\beta \chi^t_{\vec{k},\vec{q}}(v) e^{-vz_m} dv , \quad (2.3a)$$

where

$$\chi^t_{\vec{k},\vec{q}}(v) = \langle T\{S^+_{\vec{k},\vec{q}}(v) S^-_{-\vec{q}}(0)\}\rangle . \quad (2.3b)$$

The equation of motion for $\chi^t_{\vec{k},\vec{q}}(v)$ is

$$\left(\frac{\partial}{\partial v} + \omega_{\vec{k}\vec{q}}\right)\chi^t_{\vec{k},\vec{q}}(v) = \langle n_{\vec{k}+\vec{q}}\rangle - \langle n_{\vec{k}}\rangle - \tfrac{1}{2}U\left\langle T\left\{\left[\sum_{\vec{q}'} A_{\vec{k},\vec{q},\vec{q}'}(v)\rho_{-\vec{q}'}(v) + \rho_{-\vec{q}'}(v) A_{\vec{k},\vec{q},\vec{q}'}(v)\right] S^-_{-\vec{q}}\right\}\right\rangle$$

$$= \langle n_{\vec{k}+\vec{q}}\rangle - \langle n_{\vec{k}}\rangle - \tfrac{1}{2}U G^{III}_{\vec{k},\vec{q}}(v) , \quad (2.4)$$

where

$$\omega_{\vec{k},\vec{q}} = \epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}}$$

and

$$A_{\vec{k},\vec{q},\vec{q}'} = S^+_{\vec{k}+\vec{q},\vec{q}+\vec{q}'} - S^+_{\vec{k}+\vec{q}+\vec{q}',\vec{q}+\vec{q}'} .$$

The second term in (2.4) is a three-particle Green's function, and is denoted by $G^{III}_{\vec{k},\vec{q}}(v)$. The energy transform of (2.4) can be written as

$$\chi^t_{\vec{k},\vec{q}}(z_m) = \chi^t_{\vec{k}}(\underline{q}) = \frac{\langle n_{\vec{k}+\vec{q}}\rangle - \langle n_{\vec{k}}\rangle}{\omega_{\vec{k}\vec{q}} + z_m} - \frac{U}{2}\frac{G^{III}_{\vec{k}}(\underline{q})}{\omega_{\vec{k}\vec{q}} + z_m} . \quad (2.5a)$$

We therefore have

$$\chi^t(\underline{q}) = \chi^{0A}(\underline{q}) - \sum_{\vec{k}} \frac{G^{III}_{\vec{k}}(\underline{q})}{\omega_{\vec{k}\vec{q}} + z_m} . \quad (2.5b)$$

B. General discussion of equation for $\chi^t_k(\underline{q})$

In Eq. (2.5b)

$$\chi^{0A}(\underline{q}) = \sum_{\vec{k}} \frac{\langle n_{\vec{k}+\vec{q}}\rangle - \langle n_{\vec{k}}\rangle}{\omega_{\vec{k}\vec{q}} + z_m} \quad (2.6)$$

is a quantity very similar to the free-electron-gas susceptibility function. The difference is that the true occupation number $\langle n_{\vec{k}}\rangle$, i.e., the occupation number influenced by the interaction, occurs in $\chi^{0A}(\underline{q})$, instead of the bare occupation number $\langle n_{\vec{k}}\rangle = f^-{}_{\epsilon_{\vec{k}}}$. We shall return to this difference later, in Sec. III. The second term, involving $G^{III}_{\vec{k}}(\underline{q})$, can be expressed diagrammatically using its definition, i.e., Eq. (2.4). Equation (2.4) specifies the momenta, spins, and energies of the incoming and outgoing lines, and also the momenta and energies to be summed over. The diagrams consist of spin-triplet and spin-singlet particle-hole scattering amplitudes Γ^t and Γ^s, connected by single-particle Green's functions. Some examples are given in Figs. 2(a)–2(d). Clearly an infinite number of diagrams constitute $G^{III}_{\vec{k}}(\underline{q})$. We describe below how the ones believed to be significant close to the phase transition are selected out of these.

Near the phase transition ($T \simeq T_c$ or the effective interaction $U_{\text{eff}} \simeq U_{\text{eff}}^{\text{critical}}$) the spin susceptibility $\chi(\vec{q}, \omega^+)$ is very large for small values of $|\vec{q}|$ and ω. Since $\chi(\vec{q}, \omega^+)$ is closely related to $\Gamma^t(q, \omega^+)$, i.e.,

$$\chi(q, \omega^+) = [\chi^{0A}(q, \omega^+)]^2 \Gamma^t(q, \omega^+) , \quad (2.7)$$

the small-q, small-ω spin-triplet particle-hole scattering amplitude is nearly singular. The spin-singlet scattering amplitude is not singular and thus one does not expect contribution to G^{III} involving only Γ^s's to be either very large or to be strongly temperature dependent. Such terms can be classed with the Pauli term $\chi^{0A}(\underline{q})$ appearing on the right-hand side of Eq. (2.5). We shall not evaluate these terms though, in principle, their value can be comparable to $\chi^{0A}(\underline{q})$. Next we consider diagrams which involve one or more Γ^t's. These can be divided into two subclasses. There is first a set of diagrams for $G^{III}_k(\underline{q})$ involving $\Gamma^t(\underline{q})$ (the momentum and energy transfer $\vec{q}$, z_m are in the particle-hole channel 13, see Fig. 1). Now since $\Gamma^t(\underline{q})$ is (very) large and behaves in nearly the same way as $\chi^t(\underline{q})$, these "coherent" [i.e., same $(\vec{q}, z_m)$] diagrams make the most significant contribution to $\chi^t(\underline{q})$. The other subclass also involves Γ^t's, but their "four-momentum" is not $\vec{q}, z_m$ (incoherent terms). In these obviously the arguments $(\vec{q}', z_{m'})$ of the Γ^t's are internal variables which are summed over. These diagrams again will not contribute significantly if such internal summations lead to nonsingular final values. We show in Sec. III that indeed

$$\sum_{\underline{q}'} \chi^t(\underline{q}') = A' + B'(k_B T \rho_{\epsilon_F})^{4/3} \tag{2.8a}$$

for a three-dimensional system, where A' and B' are constants of order unity. Therefore such incoherent triplet terms can be grouped together with the Pauli and singlet terms discussed above, and all of these taken together constitute the interaction-renormalized, weakly temperature-dependent inhomogeneous term in the Eq. (2.6) for $\chi^t(\underline{q})$. For simplicity, we approximate this by $\chi^{0A}(\underline{q})$.

We now discuss the coherent term in more detail. As mentioned above, the coherent term is the collection of all diagrams for $G_{\vec{k}}^{\text{III}}(\underline{q})$ involving $\Gamma^t(\underline{q})$. Some examples are shown in Fig. 2(a)–2(d). The simplest coherent diagram is the RPA term, in which, for $G^{\text{III}}{}_{\vec{k},\vec{q}}(v)$, one creation and one annihilation operator at time v are joined to each other, and the remaining creation and annihilation operators form ingoing and outcoming (particle and hole) lines of the spin triplet scattering amplitude $\Gamma^t(\underline{q})$. A diagram of this type is shown in Fig. 2(a). Collecting all diagrams of this type together we find that their value is

$$\{G_{\vec{k}}^{\text{III}}(\underline{q})\}^{\text{RPA}} = -2\{\langle n_{\vec{k}+\vec{q}}\rangle - \langle n_{\vec{k}}\rangle\}\chi^t(\underline{q}) . \tag{2.9}$$

This is exactly the term retained by Izuyama, Kim, and Kubo[2] in a Green's-function decoupling scheme.

The remaining coherent diagrams have one $\Gamma^t(\underline{q})$ and one or more spin-triplet or -singlet scattering amplitudes. The momentum and energy transfers involved in these additional, internal Γ^t, Γ^s are summed over. Consider first diagrams where only internal Γ^s's are involved. Since nothing special happens to Γ^s near the ferromagnetic instability, the coefficient multiplying $\Gamma^t(\underline{q})$ due to such diagrams will be only weakly temperature dependent. It is obviously difficult to estimate this coefficient, but its effect can be absorbed, for small values of $(\vec{q}, z_m)$, by redefining U. Now consider diagrams with one or more internal Γ^t's (Figs. 2(b)–2(d), for example). If they are retained, clearly, from Eq. (2.6), their contribution will have to be determined self-consistently. We shall do this below in the one-internal-spin-fluctuation or mean-fluctuation-field approximation (MFFA) (Sec. III). The result is that near T_c

$$(\chi^{-1}\chi_P)_{\text{one isf}} \propto \sum_{\underline{q}'} \Gamma^t(\underline{q}') \approx A + B(k_B T \rho_{\epsilon_F})^{4/3}, \tag{2.8b}$$

where A and B are constants of order unity (B is positive). The zero-point term A can again be absorbed in a redefinition of U, changing it to U_{eff}. The leading temperature-dependent term is $B(k_B T\rho_{\epsilon_F})^{4/3}$ and represents the significant temperature-dependent corrections to $\chi(T)$ due to spin fluctuations. In the remainder of this section, we obtain and write down the contribution of all coherent diagrams with one internal spin fluctuation (MFF terms).

C. Mean-fluctuation-field approximation

Two MFF terms are shown in Figs. 2(b) and 2(c). Their contributions to $G_{\vec{k}}^{\text{III}}(\underline{q})$ are, respectively,

$$\left[\sum_{\underline{q}} \Gamma^t(\underline{q}+\underline{q}')\phi(\underline{q}+\underline{q}',\underline{q}') \times \left(1/\beta \sum_{\nu_l} G_{\underline{k}+\underline{q}} G_{\underline{k}-\underline{q}'}\right)\right] \Lambda^t(\underline{q}) \tag{2.10a}$$

and

$$\frac{1}{2}\sum_{\underline{q}'\underline{k}'} G_{\underline{k}'} G_{\underline{k}'+\underline{q}'} G_{\underline{k}'+\underline{q}+\underline{q}'}[\Gamma^t(\underline{k}'+\underline{q}'-\underline{k}) - \Gamma^s(\underline{k}'+\underline{q}'-\underline{k})] \times \left(\frac{1}{\beta}\sum_{\nu_l} G_{\underline{k}+\underline{q}} G_{\underline{k}-\underline{q}'}\right)\Lambda^t(\underline{q}) . \tag{2.10b}$$

In Eq. (2.10a),

$$\phi(\underline{q}+\underline{q}',\underline{q}') = \sum_{\underline{k}} G_{\underline{k}} G_{\underline{k}+\underline{q}'} G_{\underline{k}+\underline{q}+\underline{q}'} , \tag{2.11}$$

where $\sum_{\underline{k}} = (1/\beta)\sum_{\nu_l}\sum_{\vec{k}}$. Further, the vertex $\Lambda^t(\underline{q})$ is defined by

$$\Lambda^t(\underline{q}) = \left\{\sum_{\underline{k}'} G_{\underline{k}'} G_{\underline{k}'+\underline{q}}\right\}^{-1} \chi^t(\underline{q}) = \left\{\sum_{\underline{k}'} G_{\underline{k}'} G_{\underline{k}'+\underline{q}}\right\} \Gamma^t(\underline{q}) . \tag{2.12}$$

Equations (2.10) and (2.12) use one of the main approximations of this paper, namely that the spin-triplet particle-hole scattering amplitude $\Gamma^t \times (\underline{p}_1, \underline{p}_2, \underline{p}_3, \underline{p}_4)$ (Fig. 1) is a sensitive function only of the four-momentum-transfer $(\underline{p}_1 - \underline{p}_3)$ in the direct particle-hole channel 13. This is physically reasonable since the static spin susceptibility, closely related to $\Gamma^t(\underline{p}_1 - \underline{p}_3 = 0)$ [see Eq. (2.7)], is very large. However, the scattering amplitude $\Gamma^t(\underline{p}_1, \underline{p}_2, \underline{p}_3, \underline{p}_4)$ is crossing symmetric, and thus may be a sensitive function also of four-momentum transfer in the crossed channel. The neglect of this crossing symmetry is one of the more serious omissions in our work. (See Sec. V).

There are 24 MFF diagrams in all for $G_{\vec{k}}^{III}(\underline{q})$, and their total contribution can be written

$$\Lambda^t(\underline{q})^{-1} G_{\vec{k}}^{III(1)}(\underline{q}) = \tfrac{1}{2} \sum_{\underline{q}'} \Lambda^t(\underline{q}') \Big\{ (1/\beta) \sum_{\nu_l} [3 G_k G_{\underline{k}+\underline{q}} (G_{\underline{k}+\underline{q}+\underline{q}'} - G_{\underline{k}+\underline{q}'}) - G_{\underline{k}+\underline{q}'} G_{\underline{k}+\underline{q}+\underline{q}'} (G_{\underline{k}} - G_{\underline{k}+\underline{q}})] \Big\}$$
$$+ \tfrac{1}{2} \sum_{\underline{q}'} \Gamma^t(\underline{q}') \Big\{ [5\phi(\underline{q}, \underline{q}') + \phi(-\underline{q}, -\underline{q}')] \Big[(1/\beta) \sum_{\nu_l} (G_{\underline{k}} G_{\underline{k}+\underline{q}'} - G_{\underline{k}+\underline{q}'} G_{\underline{k}+\underline{q}-\underline{q}'}) \Big] \Big\} . \qquad (2.13)$$

Because the coherent term for $G_{k}^{III}(\underline{q})$ is proportional to $\Lambda^t(\underline{q})$, it is convenient to define a factor

$$F_{\vec{k}}(\underline{q}) = G_{\vec{k}}^{III}(\underline{q}) \left(\Lambda^t(\underline{q}) \sum_{\underline{p}} G_{\underline{p}} G_{\underline{p}+\underline{q}} \right)^{-1} . \qquad (2.14)$$

In terms of $F_{\vec{k}}(\underline{q})$, the equation for $\chi_{\vec{k}}^t(\underline{q})$ can be written

$$\chi_{\vec{k}}^t(\underline{q}) = \frac{\chi^{0A}(\underline{q})}{1 - \frac{1}{2} U \sum_{\vec{k}} [F_{\vec{k}}(\underline{q}) / (\omega_{\vec{k}\vec{q}} + z_m)]} . \qquad (2.15)$$

In this section, we have essentially attempted an expansion of $F_{\vec{k}}(\underline{q})$ in powers of the spin-fluctuation amplitude. We have

$$F_{\vec{k}}^{(0)}(q) = F_{\vec{k}}^{RPA}(q) = 2(\langle n_{\vec{k}} \rangle - \langle n_{\vec{k}+\vec{q}} \rangle) . \qquad (2.16)$$

The right-hand side of Eq. (2.13) is $F_{\vec{k}}^{(1)}(\underline{q}) \times (\sum_{\underline{p}} G_{\underline{p}} G_{\underline{p}+\underline{q}})$. In Sec. IV, we shall discuss $F_{\vec{k}}^{(2)}(\underline{q})$ and $F_{\vec{k}}^{(3)}(\underline{q})$.

D. Self-energy

There is, in addition to (2.13), another term for $\chi^t(\underline{q})$. This arises from the RPA term (2.9) which contains the true occupation numbers $\langle n_{\vec{k}} \rangle$ and $\langle n_{\vec{k}+\vec{q}} \rangle$. These will be affected by spin fluctuations. Theoretically, one calculates the irreducible single-particle self-energy $\Sigma_{\vec{k}}(\nu_l)$ in the presence of coupling to spin fluctuations (Fig. 4). The expression for $\Sigma_{\vec{k}}(\nu_l)$ according to Fig. 4 is

$$\Sigma_{\vec{k}}(\nu_l) = \tfrac{3}{2} \sum_{\underline{k}'} \Gamma^t(\underline{k} - \underline{k}') G_{\vec{k}'}(\nu_{l'}) . \qquad (2.17)$$

The most significant temperature-dependent part is to be extracted out of $\Sigma_{\vec{k}}(\nu_l)$ and thence $\langle n_{\vec{k}} \rangle$. We do this in Sec. III, and show that this self-energy contribution to $\chi(\underline{q})^{-1}$ is qualitatively and quantitatively similar to that of $F_{\vec{k}}^{(1)}(\underline{q})$. In contrast, for superconductors, the self-energy term is larger by a factor $(T_F/T_c)^2$.

III. EVALUATION OF MEAN-FLUCTUATION-FIELD TERM

A. Analytical results

The mean-fluctuation-field term (2.13) is quite complicated in appearance and cannot be evaluated without further approximation. The first approximation made is that bare single-particle propagators are used instead of true propagators. Since we are mainly interested in the temperature dependence of physical quantities, the approximation is reasonable if no significant temperature-dependent terms are omitted as a consequence. We show below that the temperature-dependent part of $\Sigma_{\vec{k}}(\nu_l)$ [See Eqs. (2.17), (3.15), and (3.17)] is proportional to $T^{4/3}$. The temperature-dependent spin-fluctuation correction term $F_{\vec{k}}^{(1)}(\underline{q})$ is itself proportional to $T^{4/3}$, and thus including the temperature dependence of $G_{\vec{k}}(\nu_l)$ will result in a negligible correction of order $T^{8/3}$. Thus the single-particle propagator is sufficiently well represented by its $T = 0$ part. We approximate this by the bare propagator. The second approximation is based on the fact that $\Gamma^t(\vec{q}, \omega^+)$ is strongly peaked near $|\vec{q}| = 0$ and $\omega = 0$. The single-particle Green's function $G_{\vec{k}}(\nu_l)$, however, varies over a scale k_F in momentum and ϵ_F in energy. So, we can make an expansion of the G factors multiplying $\Gamma^t(\underline{q}')$ in powers $|\vec{q}'|$ and ω'. Detailed calculation shows that it is necessary only to retain the $|\vec{q}'| = 0$, $\omega' = 0$ term to obtain the leading temperature dependence. With the above approximations, Eq. (2.13) is easily simplified, and we have

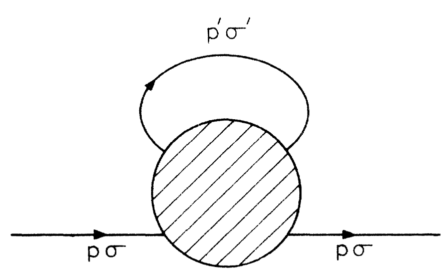

FIG. 4. Diagram for the irreducible self-energy Σ_p.

$$\sum_{\vec{k}} \frac{F_{\vec{k}}^{(1)}(\underline{q})}{\omega_{\vec{k}\vec{q}}+z_m} = -\lambda \sum_{\underline{q}'} \chi^t(\underline{q}'), \tag{3.1}$$

where

$$\lambda = -\tfrac{1}{3}U(\rho''\rho^{-2} - 9\rho'^2\rho^{-3}). \tag{3.2}$$

In (3.2), $\rho(\epsilon) = \rho$ is the density of electronic states, and the derivatives [as well as $\rho(\epsilon)$] are evaluated at $\epsilon = \epsilon_F$. In writing the Eq. (3.2) we have used the identities

$$\sum_{\underline{p}} (G_{\underline{p}}^0)^3 = \tfrac{1}{2}\rho', \qquad \sum_{\underline{p}} (G_{\underline{p}}^0)^4 = -\tfrac{1}{6}\rho''. \tag{3.3}$$

Using (3.1) and (2.15) the spin susceptibility function $\chi^t(\underline{q})$ can be written

$$\chi^t(\underline{q}) = \frac{\chi^{0A}(\underline{q})}{1 - U\chi^{0A}(\underline{q}) + \lambda\sum_{\underline{q}'}\chi^t(\underline{q}')} \tag{3.4}$$

In order to obtain an explicit expression for $\chi^t(\underline{q})$, Eq. (3.4) has to be solved self-consistently. We do this below.

In order to calculate $\sum_{\underline{q}'}\chi^t(\underline{q}')$ the explicit dependence on q' and ω' is needed. From Eqs. (2.15) and (2.16) we see that it is determined by $\chi^{0A}(\vec{q}, \omega^+)$. This Lindhard function has a fairly complicated dependence on its arguments. But for $q \ll k_F$ and $(\omega/qv_F) \ll 1$ we have

$$\chi^{0A}(\vec{q}, \omega^+) = \sum_{\vec{k}} \frac{\langle n_{\vec{k}}\rangle - \langle n_{\vec{k}+\vec{q}}\rangle}{\omega_{\vec{k}\vec{q}} + \omega^\pm} = \rho^A\left(1 - \delta q^2 \pm i\gamma\frac{\pi\omega}{qv_F}\right). \tag{3.5}$$

The small $|\vec{q}|$ and ω region is obviously the most important. We therefore use the form (3.5), assuming it to be valid throughout. The error thus introduced is not large. With the approximation (3.5) and $\rho^A = \rho_{\epsilon_F} = \rho$ (see Sec. III B) Eq. (3.2) becomes

$$\chi^t(\vec{q}, \omega^+) = \chi_P[\alpha(T) + \delta q^2 \mp i(\pi\gamma\omega/qv_F)]^{-1}, \tag{3.6}$$

where

$$\alpha(T) = [1 - U_{\text{eff}}\,\rho + \lambda\sum_{\underline{q}'}\chi^t(\underline{q}')]. \tag{3.7}$$

In order to obtain $\alpha(T)$, we have to calculate $\sum_{\underline{q}'}\chi^t(\underline{q}')$ using (3.6). This is done below.

The energy integration in $\sum_{\underline{q}}\chi^t(\underline{q})$ is easily carried out. We have

$$\frac{1}{\beta}\sum_{z_m}\chi^t(\vec{q}, z_m) = \frac{\chi_P}{\pi}\int_{-\infty}^{+\infty} d\omega\left(\frac{\gamma(\omega/qv_F)}{(\alpha+\delta q^2)^2 + \gamma^2(\omega/qv_F)^2}\right) \times (e^{\beta\omega} - 1)^{-1}. \tag{3.8}$$

The integral (3.8) can be split up into two parts, a zero-point part and a thermal part. The former is given by

$$\left(\frac{1}{\beta}\sum_{z_m}\chi^t(\vec{q}, z_m)\right)_{\text{zero pt}} = \frac{\chi_P}{\pi}\int_0^\infty \frac{(\gamma\omega\pi/qv_F)\,d\omega}{(\alpha+\delta q^2)^2 + (\gamma\omega\pi/qv_F)^2}. \tag{3.9}$$

The upper limit of integration in this term is actually $(\omega/qv_F) \approx 1$ and thus the term is convergent. This term is only weakly dependent [through $\alpha(T)$] on temperature. The term is positive and thus for positive λ, inhibits ferromagnetism. As stated earlier (Sec. I) its effect can be absorbed in U_{eff}. The thermal or temperature-dependent term is

$$\left(\frac{1}{\beta}\sum_{z_m}\chi^t(\vec{q}, z_m)\right)_{\text{therm}} = \frac{\chi_P}{\pi}\int_0^\infty \frac{(\gamma\omega\pi/qv_F)(e^{\beta\omega}-1)^{-1}}{(\alpha+\delta q^2)^2 + (\gamma\omega\pi/qv_F)^2}\,d\omega \tag{3.10}$$

$$= \frac{\chi_P}{\pi}C_q^{-1}[\ln y - (2y)^{-1} - \psi(y)], \tag{3.11}$$

where

$$C_q = (\gamma\pi/qv_F), \quad y = [\alpha(T) + \delta q^2](2\pi k_B T C_q)^{-1}.$$

$\psi(y)$ is the digamma function. We need the sum of (3.11) over all values of q. A very good approximation for $[\ln y - (2y)^{-1} - \psi(y)]$ is $(2y + 12y^2)^{-1}$. Using this, the integration over q can be carried out. The resulting expression is rather complicated and depends mildly on the upper q cutoff q_c. Defining $\bar{\delta} = \delta/k_F^2$ and $b = \pi^2\gamma k_B T/3k_F v_F\bar{\delta}$, the integral simplifies for $\frac{1}{3}\alpha(T)/\bar{\delta}b^{1/3} \ll 1$, and $q_c b^{-1/3} \gtrsim k_F$. Both these conditions can be expected to be well satisfied if $k_B T\rho \ll 1$ and $\alpha(T)$ is small, i.e., for a degenerate itinerant-electron gas not far from T_c. Then the quantity $\sum_{\underline{q}}\chi^t(\underline{q})$ has the value

$$\sum_{\underline{q}}\chi^t(\underline{q}) = k_B T\rho\bar{\delta}^{-1}\left[\frac{\pi}{\sqrt{3}}b^{1/3} - \frac{3}{2}\left(\frac{\alpha(T)}{\bar{\delta}}\right)^{1/2}\tan^{-1}\tilde{q}_c\left(\frac{\bar{\delta}}{\alpha(T)}\right)^{1/2}\right]. \tag{3.12}$$

In Eq. (3.12), $\tilde{q}_c = (q_c/k_F)(k_B T\rho)^{1/3}$. We notice that the amplitude of thermal spin fluctuations is roughly proportional to $(k_B T\rho)^{4/3}$. This is qualitatively understood as follows. $(k_B T\rho)$ is the relative volume in energy space of fluctuations with energy less than k_BT, this cutoff arising from the thermal occupation factor $(e^{\beta\omega}-1)^{-1}$. The volume in q space of these fluctuations contributes a further factor $(k_BT\rho)^{1/3}$. Using Eqs. (3.7) and (3.12) $\alpha(T)$ can now be calculated self-consistently. Before proceeding to the actual calculation, we evaluate the temperature-dependent contribution of the self-energy term.

B. Self-energy correction

In the RPA term (2.9), and its approximate form (3.5), we see that

$$\rho^A = -\sum_{\vec{k}} \left(\partial\langle n_{\vec{k}}\rangle/\partial\epsilon_{\vec{k}}\right) \tag{3.13}$$

will depend on temperature through the spin-fluctuation amplitude. We have

$$\begin{aligned}\langle n_{\vec{k}}\rangle &= \frac{1}{\beta}\sum_{\nu_l} G_{\vec{k}}(\nu_l) \\ &= \frac{1}{\beta}\sum_{\vec{k}} G^0_{\vec{k}}(\nu_l)[1+\Sigma_{\vec{k}}(\nu_l)G^0_{\vec{k}}(\nu_l)+\cdots]\,.\end{aligned} \tag{3.14}$$

It is enough to retain the term proportional to Σ for evaluating the leading temperature-dependent correction. Using the expression (2.17) for $\Sigma_{\vec{k}}(\nu_l)$ in (3.14) we find that

$$\rho^A = \rho^0\left[1-\tfrac{3}{2}\rho''\rho^{-2}\left(\sum_{\underline{q}} \chi^t(\underline{q})\right)_{\text{therm}}\right]. \tag{3.15}$$

This leads to a self-energy contribution

$$\lambda_{se} = -\tfrac{3}{2}U\rho''^2\rho^{-2} \tag{3.16}$$

to λ (Eq. 3.2).

C. Numerical results for Ni

We now numerically evaluate $\alpha(T)$ [Eqs. (3.6) and (3.7)] and thence $\chi(T)$ for Ni. The band-structure parameters needed are n_h, ρ, ρ', ρ'', δ, and γ. These are not accurately known. Various band-structure calculations differ considerably in their estimates.[12] The quantities ρ^n actually occur as $-\int_{-\infty}^{+\infty}\rho^n(\epsilon)f_\epsilon^{-\prime}\,d\epsilon$. Since the density of states $\rho(\epsilon)$ and its derivatives vary rapidly as a function of energy, $-\int_{-\infty}^{+\infty}\rho^n(\epsilon)f_\epsilon^{-\prime}\,d\epsilon$ may not equal $\rho^n(0)$ and may depend on temperature. We ignore this possibility. The constants δ and γ are even less reliably known. Lowde and Windsor[12] have calculated the Lindhard function for Ni, using the band structure results of Hubbard and Dalton.[12] We take for our constants values which are consistent with these results. We take $\rho=1.6$ states/(eV atom spin) and $n_h=0.8$ per atom. We also choose $\delta=1$, $\gamma=2$, $\rho''/\rho^3=-0.5$, $\rho'/\rho^2=0.4$. From the observed T_c, $k_BT_c\rho=0.087$ and with these parameters $1-U_{\text{eff}}\rho=0.2$. The value of $\chi(T)^{-1}\chi_P$, i.e., of $\alpha(T)$, is plotted in Fig. 3 as a function of $k_BT\rho$. We see that our results agree well with experimental values[13] over a relatively wide range of temperatures $0.10\lesssim k_BT\rho\lesssim 0.15$. In view of the uncertainty in the constants and the consequent flexibility, the agreement with experiment may not be very surprising. However, the following points need to be noted. The agreement is not greatly impaired by small adjustments in the constants. It is good over a wide range of temperatures, i.e., from 1.1 to 1.7 T_c. There is a definite dip in $\chi^{-1}(0,0)$ very close to T_c. These qualitative features are independent of the constants used. We shall see in the next section that higher-order contributions to χ^{-1} become large in the temperature range $0.09\lesssim T_c\lesssim 0.1$ and fill up this dip. The temperature-dependent part of the Stoner term is $\frac{1}{6}\pi^2(k_BT\rho)^2(\rho''/\rho^3)$. Evaluation with the parameters given above shows this term to be very small, nearly 5% of the spin-fluctuation term discussed in detail above. This is to be expected, since the Stoner term is qualitatively smaller by a factor $(k_BT\rho)^{-2/3}\sim 5$. Other coefficients contribute a further factor of 4. We thus see that the Stoner or RPA term is too small to explain the temperature dependence of $\chi(T)$, which is conventionally fitted to a Curie-Weiss formula $\chi(T)=C/(T-\Theta)$. The MFFA leads analytically to an approximate form [see Eqs. (3.7) and (3.12)]

$$[\chi^{-1}(T)\chi_P]\simeq A(k_BT\rho_{\epsilon_F})^{4/3}-B\,, \tag{3.17}$$

where A and B are known constants. This is close to a Curie-Weiss-like dependence provided T is not too far away from T_c. The self-consistent numerical solution of Eqs. (3.7) and (3.12) differs from Eq. (3.17), especially near T_c and describes the observed $\chi(T)$ quite well in the range $0.10 < T_c\rho_{\epsilon_F} < 0.16$.

D. Two-dimensional systems

We conclude Sec. III with a calculation of the static spin susceptibility for a two-dimensional system, in the mean-fluctuation-field approximation. The calculation illustrates clearly the effect of spin fluctuations in destroying ferromagnetism in one- and two-dimensional systems. We evaluate the susceptibility using the self-consistent equation (3.7) for $\alpha(T)=\chi(0)^{-1}\chi_P$. The only qualitative difference from the three-dimensional case discussed before is in the momentum summation on the right-hand side of Eq. (3.7), which is now over a two-dimensional space. The result of energy summation and momentum summation in Eq. (3.7) can be well simulated by keeping only the $z_{m'}=0$ term in the right-hand side of Eq. (3.7) and having a q' cutoff $q_c' \simeq k_F(k_B T\rho_{E_F})^{1/3}$. The reason for this is the following. If the energy summation is carried out, the Bose factor $(e^{\beta\omega'}-1)^{-1}$ effectively restricts the contributions to those from spin fluctuations of energy $\omega' \sim k_B T$. Thus in a discrete sum over $z_{m'}$, the terms of which are spaced $\sim k_B T$ apart, it may be sufficient to retain only the $z_{m'}$ (or m') = 0 term. Now spin fluctuations of energy $\omega' \sim k_B T$ have characteristic $q' \sim k_F(k_B T\rho_{E_F})^{1/3}$. Thus, a consistent approximation for thermal spin fluctuations is to consider only the $z_{m'}=0$ term and take $q_c' \simeq k_F(k_B T\rho_{E_F})^{1/3}$. One can, in fact, obtain the result of Eq. (3.12) by this approximation, which may be called the classical (statistical mechanics) approximation for the spin fluctuations. We now use this simple approximation to calculate $\alpha_{2d}(T)=\chi_{2d}(T)^{-1}\chi_P$ for a two-dimensional system using Eq. (3.7) and find

$$\alpha(T)=1-U_{\text{eff}}\rho^{0A}+(k_B T\rho\lambda/2\bar\delta)\ln(1+\bar\delta b^2\alpha(T)^{-1}). \tag{3.18}$$

It is clear from (3.18) that we cannot consistently have $\alpha(T)\to 0$, i.e., the effect of the last (one-spin-fluctuation) term in Eq. (3.18) is to suppress the ferromagnetic instability. We have calculated $\chi(T)$ for a substance with the band parameters of Ni (Fig. 4). This calculation has some meaning, since the density of states, etc. depend largely on the short-range disposition of Ni atoms. So the band parameters of a thin film may not be very different from those of the bulk. We see that at high temperatures, i.e., T between 1.5 and 2 T_c^{3d}, $(\chi^{-1})^{2d}$ is fairly close to $(\chi^{-1})^{3d}$, though somewhat less than it. As T approaches T_c^{3d} $(\chi^{-1})^{2d}$ decreases but not very rapidly. The behavior of χ^{-1} at very low temperatures cannot be reliably estimated in the MFFA, since spin-fluctuation interaction effects become important then. It is unlikely that higher-order fluctuation effects make χ singular at $T\neq 0$. No experimental susceptibility results on two-dimensional films are known, but in intercalated Mo compounds[14] with large interlayer separations, $\chi(T)$ starts off at high-temperature being Curie-Weiss like, but then slowly curves parallel to the temperature axis. The behavior is not dissimilar to that shown in Fig. 3.

IV. HIGHER-ORDER TERMS

We now investigate the effect of coherent diagrams with more than one internal spin fluctuation. It can be shown that in the classical limit,[15] for $|\vec q|\to 0$, the contribution of two internal spin fluctuation diagrams to $[\chi^t(\underline{q})]^{-1}$ vanishes identically. Their contribution is negligibly small for small $|\vec q|$ and ω. The first significant correction thus arises from the three-spin-fluctuation term [Fig. 2(d)]. Three-spin-fluctuation terms in which the fluctuations are uncorrelated contribute to $\chi^t(\underline{0})^{-1}$ a quantity of the type

$$[\chi_\rho\chi^t(\underline{0})^{-1}]^{(3)}=[A+B(k_B T\rho)^{4/3}]^3 .$$

This clearly leads to corrections to U, to the size of the thermal MFF term, and to negligible higher-order corrections of order $(k_B T\rho)^{8/3}$ and $(k_B T\rho)^4$. The effect of the first is absorbed in the redefinition of U_{eff}. The effect of the second correction is also to some extent included if U is replaced by U_{eff}. There is, however, a remaining effect which we are unable to estimate. To this extent, our estimate of λ is not exact.

The qualitatively different three-spin-fluctuation diagrams are those like Fig. 2(d) in which there is a correlation between fluctuations. Considering both longitudinal and transverse intermediate spin fluctuations, we find that

$$\sum_{\vec k}\frac{F^{(3)}_{\vec k}(\underline{q})}{(\omega_{\vec k\vec q}+z_m)}=[\chi^t(\underline{q})^{-1}]^{(3)}\chi_P = \tfrac{7}{36}U_{\text{eff}}\rho''^2\sum_{\underline{q}_1,\underline{q}_2}\Gamma^t(\underline{q}_1)\Gamma^t(\underline{q}_2) \times\Gamma^t(\underline{q}-\underline{q}_1-\underline{q}_2). \tag{4.1}$$

One limiting case of interest is $z_m\to\omega^+\to 0$ (static limit). If q also tends to zero, this gives us the three-spin-fluctuation contribution to static spin susceptibility. The quantity of interest is the temperature-dependent part. This is most simply obtained in the classical limit,[15] and leads to

$$(\Delta\chi^{-1})^{(3)}\chi_P=\frac{7}{36}U_{\text{eff}}(k_B T\rho)^2(\rho''\rho^{-3})^2 \times\sum_{\vec q_1,\vec q_2}\frac{1}{\alpha+\delta q_1^2}\,\frac{1}{\alpha+\delta q_2^2}\,\frac{1}{\alpha+\delta(\vec q_1+\vec q_2)^2}. \tag{4.2}$$

This is[16]

$$(\Delta\chi^{-1})^{(3)}\chi_P=\alpha^{(3)}(T)=U_{\text{eff}}\rho(\tfrac{7}{128}\pi^2)(\rho''^2\rho^{-2}k_B T)^2 \times\bar\delta^{-3}\ln[b^2\bar\delta/\alpha(T)]. \tag{4.3}$$

The general effect of this term is to increase $\chi^{-1}(T)$ over the MFF value, especially for T close to T_c. This will improve agreement with experiment. For the case of nickel (Sec. III B) $\alpha^{(3)}(T)\simeq\alpha^{(1)}(T)$ for $\epsilon=(T-T_c)/T_c=0.05$. We are then well in the critical regime where fluctuation interactions are quite important. This estimate accords well with experiment.[13]

One can similarly calculate the effect of spin-fluctuation interactions on the dynamic spin susceptibility. The first significant term arises from Eq. (4.1). The imaginary part of this for small values of q is proportional to ω and is given by

$$[\mathrm{Im}\chi(q,\omega^+)^{-1}]^{(3)} = (7I/32\pi^2)(k_B T\rho''\rho^{-2})^2\, U_{\mathrm{eff}}\rho\gamma\bar{\delta}^{-5/2}\alpha^{-3/2}(\omega\rho). \tag{4.4}$$

In Eq. (4.4), I is an integral of order 5. In the calculation of Eq. (4.4) we have assumed that $\mathrm{Im}[\chi^t(q,\omega^+)]^{-1} = \pi\gamma\omega/qv_F$, i.e., the collisionless RPA value (Eq. 3.5). Therefore, when Eq. (4.4) becomes comparable to $\pi\omega\gamma/qv_F$, we are in the collision-dominated critical regime. Again for Ni, this happens for $\epsilon = (T - T_c)/T_c = 0.06\, q/k_F$. Thus the size of the dynamic critical regime depends on the q value for which $\mathrm{Im}[\chi^t(q,\omega^+)]^{-1}$ is measured. In neutron scattering, q is large, $\approx 0.3\, k_F$ and $\epsilon \approx 0.02$.[17] However, in some experiments,[18] the quantity

$$\tau_{zz} = \lim_{\omega\to 0} \sum_q \omega^{-1}\,\mathrm{Im}[\chi^t(q,\omega^+)]$$

is measured. From the above result it is clear that as ϵ decreases, there is a decreasing nonhydrodynamic region in q space around $q = 0$. Thus $\tau_{zz}(\epsilon)$ may not obey dynamic scaling. Experimentally, it does not.

V. CONCLUSION AND DISCUSSION

In the work described above, we have tried to obtain from microscopic theory the effect of spin fluctuations on the spin susceptibility function $\chi(\vec{q},\omega^+)$. The temperature dependence of this contribution was found to dominate the temperature dependence of χ for small $|\vec{q}|$ and ω, and for T near T_c. One effect of spin fluctuations (of the zero-point part of spin fluctuations) is to modify the Stoner criterion, i.e., modify U to U_{eff}. This was not evaluated. It was then shown that there is a $T^{4/3}$ term in the one-spin-fluctuation contribution. The coefficient of this was evaluated in the MFFA (Sec. III) and the observed Curie-Weiss law was explained using the MFF term, a comparison being made with Ni. There are $T^{4/3}$ contributions from other diagrams [e.g., diagrams with one $\Gamma^t(q)$, plus one or more internal Γ^t's, and one or more internal Γ^s's]. Thus the MFFA coefficient represents an approximate estimate. In Sec. IV, we showed how fluctuation interactions take one into the critical regime. We now compare our results with earlier work on this problem and discuss the application of these ideas to related problems.

An equation similar to (3.4) has also been obtained by Moriya and Kawabata.[7] They assume that the RPA expression for $\chi^t(\underline{q})^{-1}$ is modified by an additive constant. This additive constant is determined by requiring that the susceptibility χ satisfy the identity $\chi = (\partial^2 F_M/\partial M^2)_{M\to 0}$, the free energy being determined as the sum of ladder and bubble diagrams. Our method is more direct and constitutes a general many-body theory for order-parameter fluctuation effects on susceptibility. As such, it can be applied to discuss a number of properties outside the purview of the Moriya-Kawabata method, for example higher-order (or critical) static and dynamic susceptibility terms (Sec. IV), effect of spin fluctuations on spin waves, fluctuations in superconductors and itinerant-electron antiferromagnets. There are also specific differences. The final value for λ (including the self-energy-term contribution, [see Eqs. (3.2) and (3.16)] is different from the Moriya-Kawabata value of

$$\lambda_{\mathrm{MK}} = -\tfrac{4}{3}\rho''\rho^{-3}\,.$$

Murata and Doniach[6] have applied a semiclassical approximation to the functional integral method and obtain a classical free energy functional suitable for describing magnetic fluctuations. Our fully microscopic method has a much wider range of applicability, as described above. For the paramagnetic phase, our results differ (e.g., there is a natural cutoff b [see Eq. (3.12)] and $\lambda_{\mathrm{MD}} = -\rho''\rho^{-3}$ is not the same as ours). Since our method is direct and enables one to systematically locate all contributions to λ we feel that our value of λ, i.e., $\lambda = -\frac{11}{6}U\rho\rho''\rho^{-3} + 3U\rho\rho'^2\rho^{-4}$, is correct.

A number of Fermi systems are nearly ferromagnetic, i.e., have large spin susceptibilities (compared to χ_P). Examples are He^3,[19] Pd,[20] Ni_3Ga,[21] $HfZn_2$,[22] etc. It is also found that their susceptibilities are strongly temperature dependent. The theory described here explains the strong temperature dependence of $\chi(T)$, if we assume $U_{\mathrm{eff}}\rho \lesssim 1$. The observed Curie-Weiss law for $\chi(T)$, with a characteristic temperature $T_F(1 - U_{\mathrm{eff}}\rho)$, is in quantitative accord with the results of MFFA (Sec. III). We had earlier explained this[23] using microscopic Fermi-liquid theory. The essential idea there is to use the fact that Γ^t is large and sensitively q and ω dependent, plus the crossing symmetry of Γ^t. The resulting temperature dependence of $\chi(T)$ is in good agreement with experiment for He^3. The work here provides an alternative dynamical explanation for the strong temperature dependence of $\chi(T)$. Crossing symmetry has not been maintained or assumed in the calculation of the MFF term. In Fermi-liquid-theory language, the dynamical model used here shows that the spin-triplet Landau parameter F_0^t is strongly temperature dependent. This effect cannot be seen in a formal microscopic Fermi-liquid theory which is based on $T=0$ parameters, and needs a dynamical model. Both the temperature dependence of F_0^t and the crossing symmetry of $\Gamma(p_1, p_2, p_3, p_4)$ are contributing factors, probably of comparable significance.

Recently, Béal-Monod[24] *et al.* have attempted to explain the temperature-dependent resistivity of some nearly ferromagnetic metals by invoking the temperature-dependent Stoner term in $\chi^{-1}(T)$. Clearly the MFF term is much more important. Its inclusion is seen to increase the range of temperatures over which agreement is obtained. It is also not necessary then to use for the Fermi temperature of the $5f$ band (known to be fairly wide) such abnormally small values as 280 °K (Pu) and 620 °K (Np).

We have extended the method to the ferromagnetic phase[10] and have obtained the longitudinal and transverse dynamic spin susceptibilities in the MFFA. The latter has poles (spin-wave poles) whose positions are shifted with respect to the Stoner value. We find in general that the spin-wave stiffness decreases due to spin fluctuations. The effect of spin fluctuations on magnetization and on thermodynamic properties is being computed. The results will be presented in a subsequent paper.

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