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Thermodynamics of an itinerant-electron ferromagnet at very low T_C/ϵ_F†

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The validity of the classical Murata-Doniach model for the thermodynamic properties of weak itinerant magnets near T_C is discussed in detail. An explicit perturbation expansion for the nontrivial thermodynamic properties in the model is carried out in terms of two small parameters available for very weak transitions. Furthermore, a microscopic examination of quantum corrections (the $\omega_n \neq 0$ modes) suggests that the classical phenomenological model with temperature-independent Ginsburg-Landau (GL) coefficients in valid as $T_C \to 0$ if the fluctuation phase space is simply restricted to the thermal population. Thus, if the excitations are paramagnons with q^3 damping, the fluctuations must be cut off at a momentum $q_m \sim T^{1/3}$. We find that the model is necessarily phenomenological in the sense that the quantum corrections enter the GL coefficients without benefit of a small parameter. However, given the coefficients, a small parameter *is* available for the Murata-Doniach model (T_C/ϵ_F) if the phase transition happens to be weak. This difficulty should be present in the similar Moriya-Kawabata approach. The coefficients could presumably be determined by detailed fitting to itinerant magnets with T_C in the 1-K region.

I. INTRODUCTION

In a previous letter, Murata and Doniach,[1] hereafter called I, proposed a fluctuation mechanism in itinerant ferromagnets which could qualitatively account for the magnitude of the Curie constant observed in low-temperature itinerant ferromagnets. Briefly, the difficulty with the random-phase approximation (RPA)[2] or Stoner-theory[3] susceptibility,

$$\chi_{\mathrm{RPA}}^{-1} \propto 1 - U\bar{N}(\epsilon_F), \tag{1.1}$$

is the weak T^2 temperature dependence introduced by the thermal average of the density of states $\bar{N}(\epsilon)$:

$$\bar{N}(\epsilon_F) = -\int d\epsilon \left(\frac{\partial f}{\partial \epsilon}\right) N(\epsilon), \\ \approx N(\epsilon_F) + \tfrac{1}{6}\pi^2 N''(\epsilon_F) T^2, \tag{1.2}$$

where f is the Fermi factor. As a consequence, although an expansion around the zero of χ_{RPA}^{-1} does give $T - T_C$ behavior over a short range, the Curie constant is enhanced by a factor ϵ_F/T_C. In very weak itinerant magnets, it is found experimentally[4] that Curie-Weiss behavior extends over a wide temperature range and that this factor should be more like unity.

The Murata-Doniach (MD) suggestion is that most of the temperature dependence in χ_{RPA} is missed and comes from local magnetization fluctuations $\langle m_i^2\rangle$ which could enter the susceptibility through a fourth-order coupling

$$\sum_i \beta m_i^4 \approx 6\beta \sum_i \left(m_i^2\langle m_i^2\rangle - \tfrac{1}{2}\langle m_i^2\rangle^2\right) \tag{1.3}$$

in the free-energy functional. Since the mean-square expectation of a *classical* field grows intrinsically as the temperature

$$\langle m_i^2\rangle = O(T), \tag{1.4}$$

such coupling could be the source of the Curie law if β is the right order of magnitude. This fluctuation coupling is in fact the mechanism for the Curie law in displacive structural phase transitions and has been understood for some time.[5]

Unfortunately, attempts to fit the thermodynamic properties in the mean-field region from the MD model [with constant Ginsburg-Landau (GL) coefficients] failed for $ZrZn_2$ ($T_C \approx 20$ K), although a qualitative fit could be obtained for Sc_3In ($T_C \sim 6$ K) for $T < 12$ K. The slope of the latter's measured inverse susceptibility,[6] however, appeared to change suddenly to a new value for $200 > T > 12$ K. This behavior and the fact that $ZrZn_2$ could not be fit to the model suggested strong temperature-dependent renormalization effects in the GL coefficients at these higher temperatures. The proper direction to go to obtain good fits to the model appeared to be to compounds with even lower transition temperatures. While there are no candidates in mind, a possibility exists that good homogeneous itinerant magnets with lower T_C will be found even though the magnetic transition is not inherently weak and a low T_C/ϵ_F is "accidental." One could alternatively perform accurate measurements on $ZrZn_2$ at pressures of order 20 kbar, which are sufficient to reduce T_C to zero.[7]

To increase interest in these possibilities, a justification of the model seems desirable at the present time. The point of this paper is (i) to demonstrate the consequences of the MD model at very low T_C from perturbation theory, and (ii) to show that it should become an exact description of the region near T_C as $T_C \to 0$. This is quite surprising because one knows that classical models break down at zero temperature. On the other hand we are claiming an improvement as $T_C \to 0$. The improvement occurs, however, within a fixed region around T_C, which shrinks in absolute range along with T_C. The improvement occurs because in general the GL coefficients are temperature dependent. The precise dependence cannot be determined because the itinerant magnet is a strong-coupling problem ($U/\epsilon_F \sim 1$), unlike, say, the superconductor. However, it is possible to estimate the temperature dependence of the GL coefficients from the microscopic theory, as we do in Sec. V, and show that this becomes negligible as $T_C \to 0$, compared to other effects, like (1.4).

Now, one other proviso has to be made. Although the GL coefficients tend to constant values (which are not known, except in order of magnitude), quantum effects come into play to freeze out the classical fluctuations as $T_C \to 0$. In Sec. V we show that this effect can be absorbed into a temperature-dependent upper cutoff q_m, at least within low-order approximations likely to be used for the MD model. The finding is that q_m should be chosen to include only the thermal population in the MD model. In the present case we are rather fortunate in that spinlike excitations become rather stiff. The best description for low-momentum spin fluctuations is probably paramagnon theory. Paramagnons become incredibly stiff, with a damping rate very close to T_C going as q^3. Within paramagnon theory, then, we expect that $q_m^3 \sim T$ or $q_m \sim T^{1/3}$, which is rather weak dependence. If high-momentum spin waves are important above T_C in the thermodynamics, which is not likely, then we should have q_m going more like $q_m \sim T^{1/2}$.

We note that it would be unreasonable if the GL coefficients could be determined from first principles, for then one could determine the nature of the transition in a dense interacting electron gas, which is known to be intractible.[8] The GL coefficients can be determined only phenomenologically and not from known band structure, contrary to what may have been implied in I. This difficulty should also manifest itself in a Moriya-Kawabata[9] approach, which produces qualitatively similar results to the present model.

Given the GL coefficients which cannot be determined except in order of magnitude, we now consider the possibility of an accidentally weak transition at very small T_C/ϵ_F. At low temperatures, the flucutations themselves become weak because of (1.4), and perturbation theory in the MD model becomes possible even when the GL coefficients themselves are not small. As mentioned briefly in I, the validity of the perturbation theory for the model depends on two small parameters T/T_0 and ϵ, the first specifying a weak transition and the second that one is not in the critical region. The first is defined in Eq. (2.8) and is the same as in I; the second, defined in Eq. (2.9), is somewhat different. Close to T_C, it has the form

$$\epsilon \approx \pi^2 T^2 / 8T_0 \left(1 + \frac{T\, d\ln q_m}{dT}\bigg|_{T_C}\right)(T - T_C) \quad .$$

In contrast to recent renormalization-group efforts, we are not interested in critical effects, as the relative size of the critical region shrinks as $T_C \to 0$. One in any case knows only the critical exponents and not the detailed variation of the thermodynamic properties in this region.

The perturbation theory for the model (2.1) has been worked out in detail, for constant GL coefficients and temperature-dependent q_m. This is a straightforward but tedious exercise. The results have been compiled in Table I, which can be used as either a detailed Ginsburg[10] criterion for the model or for detailed fitting of the thermodynamic behavior. The thermodynamic behavior can be reconstructed from this table by inserting the correction terms (C.T.) into the appropriate place in the listed equation. We show how this is done. If one were to put these terms in place, the susceptibility for $T > T_C$ in Eq. (3.16) acquires the form

$$\chi_s = \frac{\mu_B^2}{U\eta_0}\left(1 - \epsilon^{1/2} + \tfrac{1}{2}\epsilon - \epsilon \ln\frac{T_0}{\Delta T} + \frac{\kappa_F \xi_0^2}{8\gamma_F^2}\, \epsilon + \cdots\right)^{-1} \quad .$$

In this equation, the first three terms come from the Hartree contribution and the last two from the Born terms and three-body contribution, respectively, as indicated in the columns of Table I. Here $\Delta T = T - T_C$. The definition of other parameters is given in Eqs. (2.1)–(2.6). For now, we want merely to indicate the type of results one obtains from the model.

The behavior of the quantity η_0 is, first, not strictly Curie-Weiss-like due to the reduction in the thermal population as $T \to 0$. In paramagnon theory, η_0 has the form $-|a| + |b|(T/\epsilon_F)^{4/3}$, with $|b|$ of order 1. In addition, the temperature dependence of the GL coefficients due to the quantum corrections, if taken into account, would introduce an additional $(T/\epsilon_F)^2 \ln(T/\epsilon_F)$ term in η_0, with a coefficient of order 1 which is calculable by solving the strong-coupling problem. Thus only at low temperatures where $(T/\epsilon_F)^{4/3} \gg (T/\epsilon_F)^2 \ln(\epsilon_F/T_C)$ does the temperature dependence predicted in the model with constant coefficients become dominant. The Curie-Weiss behavior is also modified by renormalization of the *critical* (very small q) fluctuations, which result in the ϵ corrections in (3.16). The ϵ and $T^{1/3}$ curvature effects can amount to 10% effects in the thermodynamic properties and are given for possible use in detailed fitting.

The classical model and the notation are first introduced in Sec. II. Section III discusses the classical model for $T > T_C$ in the Hartree approxi-

TABLE I. Corrections from higher-order approximations as they would enter various equations, compared to the first term from the Hartree approximation comparable to the Born and three-body corrections. The model and notation are given in Eqs. (2.1)–(2.9). To reduce the complexity of the entries, various small parameters have been ranked according to $\beta_F T\xi \gg \eta_0$: $T/T_0 \gg \epsilon^{3/2}$. The weak temperature dependence (2.11) of α_F, if included, would introduce corrections with coefficients of order of the Hartree entries in this table, times $\ln(\epsilon_F/T)$, except for the susceptibility for $T<T_C$, where the coefficient is order ϵ, not $\epsilon^{1/2}$. Here κ is of order 1 and defined following Eq. (4.19); $\Delta T = T - T_C$.

	Hartree correction	Born correction	Three-body correction
Specific heat $T>T_C$, Eq. (3.12)	$\frac{1}{2}\pi^2 \frac{T}{T_0}$	$-\frac{1}{32}\kappa\pi^2\frac{T}{T_0}+\frac{1}{4}\epsilon^{3/2}\ln\frac{T_0}{\Delta T}$	$\frac{\pi^2\kappa_F\xi_0^2}{8\gamma_F^2}\frac{T}{T_0}$
Specific heat $T>T_C$, Eq. (4.21)	$-\frac{1}{4}\pi^2\frac{T}{T_0}$	$\frac{1}{32}\pi^2(9+\frac{1}{2}\kappa)\frac{T}{T_0}+\frac{\epsilon^{3/2}}{4(2)^{1/2}}\ln\frac{T_0}{\Delta T}$	$-\frac{\pi^2\kappa_F\xi_0^2}{32\gamma_F^2}\frac{T}{T_0}$
Susceptibility $T>T_C$, Eq. (3.16)	$\frac{1}{2}\epsilon$	$-\epsilon\ln\frac{T_0}{\Delta T}$	$\frac{\kappa_F\xi_0^2}{8\gamma_F^2}\epsilon$
Susceptibility $T<T_C$, Eq. (4.13)	$(\frac{1}{2}\epsilon)^{1/2}$	$-\frac{3\epsilon^{1/2}}{2(2)^{1/2}}+\epsilon\ln\frac{T_0}{\Delta T}$	$-\frac{\kappa_F\xi_0^2}{8\gamma_F^2}\epsilon$
Magnetization Eq. (4.17b), $T>T_C$	$\frac{1}{2}\epsilon$	$-\epsilon\ln\frac{T_0}{\Delta T}$	$\frac{\kappa_F\xi_0^2}{\gamma_F^2}\epsilon$
Magnetization Eq. (4.17c), $T>T_C$	$-\frac{3}{16}\epsilon^{3/2}$	$\frac{9}{2}\epsilon-\frac{3}{4}\epsilon^{3/2}\ln\frac{T_0}{\Delta T}$	$\frac{\pi^2\kappa_F\xi_0^2}{16\gamma_F^2}\frac{T}{T_0}$
Magnetization Eq. (4.12b), $T>T_C$	$\frac{1}{4}\epsilon$	$-\frac{3}{8}\epsilon+\epsilon\ln\frac{T_0}{\Delta T}$	$-\frac{\kappa_F\xi_0^2}{8\gamma_F^2}\epsilon$
Magnetization Eq. (4.12c), $T<T_C$	$\frac{3}{64(2)^{1/2}}\epsilon^{3/2}$	$\frac{3}{16}\epsilon$	$-\frac{\pi^2\kappa_F^2\xi_0^2}{16\gamma_F^2}\frac{T}{T_0}$

mation. Section IV outlines the perturbation expansion in a field and for $T<T_C$. Corrections beyond the Hartree approximations are introduced from a variational procedure. Finally, in Sec. V, a discussion of the effects of lowest-order dynamic corrections on the model coefficients is given.

II. MODEL

The model assumes that the thermodynamics near T_C is given by a classical field functional of the form

$$\mathfrak{F}=\frac{1}{2}\sum_{q}^{q_m}|h_q|^2(\alpha_F-1+\mu_F^2q^2)-h_{q=0}\tilde{H}+\tfrac{1}{2}\tilde{H}^2+\frac{\beta_F\tilde{T}}{4!N}\sum_{\{q\}}^{q_m}h_{q_1}h_{q_2}h_{q_3}h_{q_4}\,\delta_{q_1+q_2+q_3+q_4,0}\ , \tag{2.1}$$

where h is a real field and satisfies $h_q=h^*_{-q}$, $\tilde{H}$ is the external applied field, and $\tilde{T}$ is the reduced temperature. We shall also consider the effects of adding to (2.1) the three-body term

$$\frac{1}{6!}\frac{\kappa_F\tilde{T}^2}{N^2}\sum_{\{q\}}^{q_m}h_{q_1}\cdots h_{q_6}\,\delta_{q_1+\cdots+q_6,0}\,. \tag{2.2}$$

The partition function is given by

$$e^W=Z/Z_0=\langle e^{-\mathfrak{F}}\rangle_0\ , \tag{2.3}$$

where

$$\langle \mathcal{O}\rangle_0=\int\frac{dh_0}{(2\pi)^{1/2}}\prod_{q>0}\frac{d^2h_q}{\pi}\ \mathcal{O}\,e^{-(1/2)\Sigma_q|h_q|^2}\,. \tag{2.4}$$

It is convenient at the present time to define parameters which appear in Table I. These are

$$\xi_0=(\Omega_a/2\pi^2\mu_F^3)\,\mu_F q_m\ , \tag{2.5}$$

$$\gamma_F=(\Omega_a/8\pi)\,\beta_F/\mu_F^3\ , \tag{2.6}$$

$$\eta_0=\alpha_F+\tfrac{1}{2}\beta_F\tilde{T}\xi_0\ , \tag{2.7}$$

where $\alpha_F<0$ and Ω_a is the unit-cell volume. Close to T_C,

$$\eta_0\approx\tfrac{1}{2}\beta_F\,\xi_0(T_C)\left(1+\tilde{T}\frac{d\ln q_m}{d\tilde{T}}\right)_{T_C}(\tilde{T}-\tilde{T}_C)\,.$$

We consider the case where the transition in (2.1) is weak and assume the existence of the small parameters

$$\tilde{T}/\tilde{T}_0\ll 1, \tag{2.8}$$

where $T_0=2\mu_F^2q_m^2/\beta_F\xi_0$ and

$$\epsilon\equiv\gamma_F^2\tilde{T}^2/\eta_0\ll 1,$$

$$\approx\pi^2T^2/8T_0\left(1+\tilde{T}\frac{d\ln q_m}{d\tilde{T}}\right)_{T_C}(T-T_C)\,. \tag{2.9}$$

For the ferromagnet, Eq. (2.1) follows from considering a functional-integral formalism for the Hubbard Hamiltonian, as discussed in the Appendix. Furthermore, *nominal* expressions for the coefficients in terms of the band structure of the conduction electrons are given in the static approximation:

$$\begin{aligned}
&\alpha_F^0 = 1 - 2U\bar{N}(\epsilon_F)\\
&\beta_F^0 = -\tfrac{1}{2}(2U)^3\bar{N}''(\epsilon_F) \geq 0\ ,\\
&(\mu_F^0)^2 = -\tfrac{1}{18}(2U)\bar{N}''(\epsilon_F)V_F^2\ ,\\
&\kappa_F^0 = -\tfrac{1}{4}(2U)^5\bar{N}^{(4)}(\epsilon_F)\ ,\\
&\tilde{H} = \mu_B H(N/UT)^{1/2},\quad \tilde{T} = T/2U,
\end{aligned} \tag{2.10}$$

where U is the Coulomb interaction of the Hubbard Hamiltonian,[11] and where the average of the density of states $\bar{N}(\epsilon_F)$ is given by (1.2). The averaged curvature $\bar{N}''(\epsilon_F)$ is similarly defined.

We summarize at this point the effects of the lowest-order dynamic corrections (discussed in Sec. V) on some of these nominal values. The results from (5.18) are that

$$\begin{aligned}
&\alpha_F = [\alpha_F^0 + \alpha_0^{(1)} + O((T/\epsilon_F)^2\ln(T/\epsilon_F))]/(1-c)\ ,\\
&\beta_F = \beta_F^0/(1-c)\ ,
\end{aligned} \tag{2.11}$$

where $\alpha_0^{(1)}$ and c (< 0) are temperature-independent numbers of order 1. In lowest order no extra temperature dependence appears in β_F, except for the $(T/\epsilon_F)^2$ dependence resulting from the thermal average $\bar{N}''(\epsilon_F)$ in (2.10). Furthermore, as we have mentioned

$$q_m \sim T^{1/3},$$

within paramagnon theory, which is the result in (5.22).

The notation in (2.1) is different from that used in I, which considered fluctuations in the magnetization m_q directly. For our purposes or working with the diagram representation it is more natural to use a unit-normalized fluctuation

$$h_q = m_q(2N/\tilde{T})^{1/2}, \tag{2.12}$$

with $\langle |h_q|^2\rangle_0 = 1$. The factorial coefficients in Eqs. (2.1) and (2.2) also correspond to standard field-theory notation. The partition function (2.3) differs from that of I in the absence of multiplicative factors of $T^{1/2}$ per mode from the change of variables, which would lead to classical $\frac{1}{2}\ln T$ terms in the free energy and the spurious Dulong and Petit contribution to the specific heat obtained in I. Aside from this, correspondence in terms of parameters μ^2, α, β of I can be obtained from the prescription

$$\mu^2 \to 2U\mu_F^2,\ \ \alpha \to 2U\alpha_F,\ \ \beta \to \tfrac{2}{3}U\beta_F\ .$$

The change in normalization introduces the explicit temperature dependence $\tilde{T}$ in the two-body term in (2.1). (This is, incidentally, the same T that occurs for each Matsubara frequency sum in the finite-temperature diagram technique.[12])

III. HARTREE APPROXIMATION FOR $T > T_C$

The effect of critical (i.e., small q) renormalization effects can be obtained within a Hartree approximation (1.3) for the β_F term in (2.1). The fluctuation average $\langle |h_q|^2\rangle$ and thermodynamic properties can be computed since only Gaussian integrals are present when (1.3) is substituted into the free energy, as discussed in I.

We write the results for the partition function from (2.1), (2.3), (2.4), and (1.3) as

$$e^W = \frac{Z}{Z_0} = \exp(\tfrac{1}{8}\beta_F\tilde{T}N\xi^2)\prod_q \tilde{D}_q^{1/2}, \tag{3.1}$$

where the Hartree susceptibility in zero field and for $T > T_C$ is

$$\tilde{D}_q = \langle |h_q|^2\rangle = (\alpha_F + \tfrac{1}{2}\beta_F\tilde{T}\xi + \mu_F^2 q^2)^{-1}. \tag{3.2}$$

The effective fraction of fluctuating modes is given by the self-consistency equation

$$\xi = \frac{1}{N}\sum_{q<q_m}\tilde{D}_q\ , \tag{3.3}$$

and the brackets by

$$\langle \mathcal{O}\rangle \equiv \langle \mathcal{O}\, e^{-\mathfrak{F}}\rangle_0 / \langle e^{-\mathfrak{F}}\rangle_0\ . \tag{3.4}$$

We show next that the free energy satisfies a stationary property $\delta W/\delta\tilde{D}_q = 0$, which simplifies the specific-heat calculation and which is also used in Sec. IV to define consistent self-energies from higher-order corrections beyond the Hartree approximation. The stationary property follows readily from inspection of (3.1) provided one uses the fact that

$$\frac{\delta}{\delta\tilde{D}_q}\sum_{q'}\ln\tilde{D}_{q'} = -\sum_q \tilde{D}_q\,\delta\tilde{D}_q^{-1}/\delta\tilde{D}_q = -\tfrac{1}{2}\beta_F\tilde{T}\xi N\ .$$

The prediction of the theory for the specific heat is readily obtained from (3.1). We use

$$\frac{C}{T} = 2\frac{dW}{dt} + T\frac{d^2W}{dT^2}\ . \tag{3.5}$$

We note that in differentiating W *once*, a cancellation occurs because of the stationary property $\delta W/\delta\tilde{D}_q = 0$. Also we note the derivative $d\xi/dT$ does not enter dW/dT. However, the q_m dependence of the upper limit of the product in (3.1) does contribute a term which looks like a temperature-dependent background. We obtain

$$C/T = \Delta C_{\rm crit}/T + C_b/T\ ,$$

where

$$\frac{\Delta C_{\rm crit}}{T} = -\frac{1}{4}\left(\frac{\beta_F}{2U}\right)\xi^2 N - \frac{T}{4}\left(\frac{\beta_F}{2U}\right)\xi\frac{d\xi}{dT}\ . \tag{3.6}$$

For $T < T_C$, the terms analogous to $\Delta C_{\rm crit}/T$ change sign and contribute to the specific-heat discontinuity. The background term C_b/T in (3.6), however, as discussed in Sec. IV C has the same form for $T > T_C$ and $T < T_C$, provided $|\eta_0| \ll \mu_F^2 q_m^2$. This condition near T_C can be rewritten as

$$\frac{|\Delta T|}{T_0(T_C)} \ll \left(1 + T\frac{d\ln q_m}{dT}\right)^{-1}_{T_C}, \qquad (3.7)$$

which is easily satisfied there. The form of C_b where (3.7) is satisfied is

$$\frac{C_b}{T} = \frac{\Omega_a}{4\pi^2}\frac{q_m^3}{T}\left\{\left(\ln\frac{1}{\mu_F^2 q_m^2}\right)\left[2T\frac{d\ln q_m}{dT} + 3\left(\frac{Td\ln q_m}{dT}\right)^2\right] - 2\left(\frac{Td\ln q_m}{dT}\right)^2\right\}. \qquad (3.8)$$

We note that if q_m has power-law behavior, $Td\ln q_m/dT$ is just a constant. For $q_m \sim T^{1/3}$, we also note that the background goes as

$$C_b/T \sim \text{const} + |\ln T|$$

and thus, has slow logarithmic variation near T_C.[13]

To calculate $\Delta C_{\rm crit}/T$, we obtain the self-consistency condition on ξ from (3.2) and (3.3), which is

$$\eta \equiv \tilde{D}_{q=0}^{-1} = \eta_0 - \eta^{1/2}\gamma_F \tilde{T} 2\pi^{-1}\tan^{-1}(\mu_F q_m/\eta^{1/2}). \qquad (3.9)$$

We look for an approximate solution of (3.9) for $\eta \ll 1$, so that[14] $\tan^{-1}(\mu_F q_m/\eta^{1/2}) \simeq \frac{1}{2}\pi$. This is given by

$$\eta \approx \eta_0 + \tfrac{1}{2}\gamma_F^2\tilde{T}^2 - \tfrac{1}{2}(4\eta_0\gamma_F^2\tilde{T}^2 + \gamma_F^4\tilde{T}^4)^{1/2}. \qquad (3.10)$$

In terms of the small parameters in (2.8) and (2.9), we obtain, from (3.10),

$$\eta \approx \eta_0[1 - \epsilon^{1/2} + \tfrac{1}{2}\epsilon - O(\epsilon^{3/2})] \quad \text{for } \epsilon \ll 1. \qquad (3.11)$$

From (3.9) and (3.11) we can easily obtain $d\xi/dT$, to find

$$\frac{\Delta C_{\rm crit}}{T} = -\frac{\beta_F \xi_0^2}{8U}\left[1 + \frac{Td\ln q_m}{dT} - \frac{\epsilon^{1/2}}{2} - \pi\left(\frac{\Delta T}{T_0}\right)^{1/2} + \text{C.T.}\right]. \qquad (3.12)$$

where we have used the definition (2.9) for T_0. This equation displays the format we shall use in conjunction with the "correction terms" in Table I. Only significant terms generated in the Hartree approximation are explicitly displayed in (3.12). Those which are comparable to others from higher-order corrections, are put into Table I.

Sufficiently far from the transition ($\epsilon \ll 1$), the important contribution to $\Delta C_{\rm crit}$ is thus negative, the magnitude of the subtraction depending on the effective number $\xi_0 \sim q_m$ of modes participating in the phase transition. The $\epsilon^{1/2}$ term in (3.12) is reminiscent of the $(T - T_C)^{-1/2}$ singularity predicted in the electron RPA.[2] We note, however, that the $\epsilon^{1/2}$ behavior is obtained only if $\epsilon \ll 1$ and does not actually dominate the specific-heat behavior.

One can readily derive expressions for the magnetization and susceptibility from differentiating (2.3). The physical magnetization per site is given by

$$\Delta n = \frac{N_\uparrow - N_\downarrow}{N} = \left(\frac{2\tilde{T}}{N}\right)^{1/2}\frac{dW}{d\tilde{H}} = \left(\frac{2\tilde{T}}{N}\right)^{1/2}(D - \tilde{H}), \qquad (3.13)$$

where $D = \langle h_{q=0}\rangle$, and the susceptibility per site is

$$\chi = \mu_B^2(\tilde{D}_{q=0} - 1)U^{-1}, \qquad (3.14)$$

where in general the cumulant part $\tilde{D}_q$ is defined as

$$\tilde{D}_q = \langle h_q h_q^*\rangle - \langle h_0\rangle^2\delta_{q,0}. \qquad (3.15)$$

The discussion of the magnetization equation is deferred until Sec. IV.

One can readily derive, however, the form of χ_S, the singular part of the susceptibility in (3.14) from Eqs. (3.9) and (3.11):

$$\chi_S = \mu_B^2/\eta U \simeq (\mu_B^2/U\eta_0)(1 - \epsilon^{1/2} + \text{C.T.})^{-1}. \qquad (3.16)$$

The behavior of χ_S has already been discussed in Sec. I.

IV. DIAGRAM EXPANSIONS AND HIGHER-ORDER CORRECTIONS

Next, for compactness, we shall discuss finite-magnetization results and higher-order corrections simultaneously. In going beyond the Hartree approximation, one does not have recourse to a thermodynamic-minimum principle, as used for example in I. However, one can insure by construction that the free energy satisfies stationary principles with respect to the order parameter and susceptibility that hold in an exact theory. The latter property $\delta W/\delta\tilde{D}_q = 0$ is not well known but was shown to hold in the Hartree approximation. These stationary principles are discussed in more detail by De Dominicus and Martin,[15] and for the most part we simply adopt their results.

It is convenient in using their method to work with diagram expansions for the free energy. The analogy of diagram expansions of (2.3) with that of field theories follows for Gaussian random variables as in (2.4) and should be well known from recent work on the renormalization group.

We generally wish to calculate the average (3.4) for some function $\mathcal{O}$ of the random variables h. We first expand $e^{-\mathfrak{F}} = 1 - \mathfrak{F} + \mathfrak{F}^2/2! + \cdots$. If $\mathcal{O}$ is a polynomial in h, then at each order in $\mathfrak{F}$ we must evaluate the product $\langle h_{q_1}\cdots h_{q_n}\rangle_0$. Of course, the average is nonzero unless the h's occur in pairs $|h_q|$,[4] quadruples $|h_q|^4$, etc. The algebra of keeping track of the occurrences of pairs, quadruples, etc., in the q sums leads naturally to a linked semi-invariant or cumulant expansion of $\langle\mathcal{O}\rangle$ in terms of cumulants M_n defined by $\ln\langle\exp[-\frac{1}{2}t(h_q + h_{-q})]\rangle_0 = \sum M_n t^n/n!$. The simplification for a Gaussian field theory is, of course, the fact that expectation value can be evaluated by completing the square, from which one sees that only $M_2 = \langle |h_q|^2 \rangle_0$ is nonzero. Thus, although quadruples and higher-order pairings generally occur, the net contribution to M_n, $n \geq 4$, vanishes. A theory with only M_2 generates standard diagram expansions and the full complications of a cumulant expansion, for example, for the Heisenberg ferromagnet, do not occur.[16]

For example, the second-order diagrams of Fig. 1 for $\langle e^{-\mathfrak{F}} \rangle_0$ itself is proportional to

$$\sum_{qq'} \langle h_q h_{-q} h_{q'} h_{-q'} \rangle_0 \, v_1(q)\, v_1(q') . \tag{4.1}$$

By noting that $\langle |h_q|^4 \rangle_0 = 2! \langle |h_q|^2 \rangle_0^2$ for $q \neq 0$ and $\langle |h_0|^4 \rangle_0 = 3 \langle |h_0|^2 \rangle_0^2$ for $q = 0$ one can write (4.1) as

$$\sum_{qq'} \langle |h_q|^2 \rangle_0 \langle |h_{q'}|^2 \rangle_0 \, v_1(q)\, v_1(q') + 2 \left(\sum_q \langle |h_q|^2 \rangle_0 v_1(q) \right)^2 ,$$

which corresponds to the first and second diagrams on the right of Fig. 1, respectively.

In analogy with a scalar-field theory, the h is equivalent to a field operator and $e^{-\mathfrak{F}}$ is equivalent to the s matrix for the interaction $H_{\text{int}} = v_1 h^2/2! + v_2 h^4/4! + v_3 h^6/6!$, with the one-body potential $v_1 = \alpha_F - 1 + \mu_F^2 q^2$, two-body potential $v_2 = \beta_F \tilde{T}$, and three-body potential $v_3 = \kappa_F \tilde{T}^2$. The bare propagator is $D_q^0 = \langle h_q h_q^* \rangle_0$. One finds that a Dyson equation and linked-cluster theorem follow in the standard way.

One complication is that one must, in general, allow for a finite $q = 0$ magnetization, proportional in the diagram theory to the anomalous average $D = \langle h_0 \rangle$. For finite D, it is well known from theories of boson systems (where D is the square root of the condensate density) that the cumulant part $\tilde{D}_q$, defined in (3.15), is composed of connected diagrams and can be written in terms of a proper self-energy Σ_q as $\tilde{D}_q = (1 - \Sigma_q)^{-1}$.

If we denote $\tilde{D}_q$ by an open wavy line and D by the line terminated with a shaded circle as in Fig. 2, then rules for diagrams are standard except for a factor of -1 for each interaction vertex v_i represented by a dot (in our convention for signs of propagators) and combinational factors of (i) $(n!)^{-1}$ is n terminated lines attached to a vertex, (ii) $(1/n!)(\frac{1}{2})^n$ is n single closed loops attach to a vertex, and (iii) $(n!)^{-1}$ if the same n propagators attach to any two vertices. These coefficients are just those encountered in theories of scalar bosons.

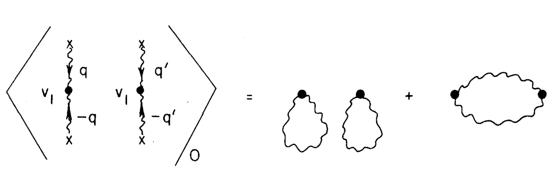

FIG. 1. Example of the diagram expansion for a term in the free energy.

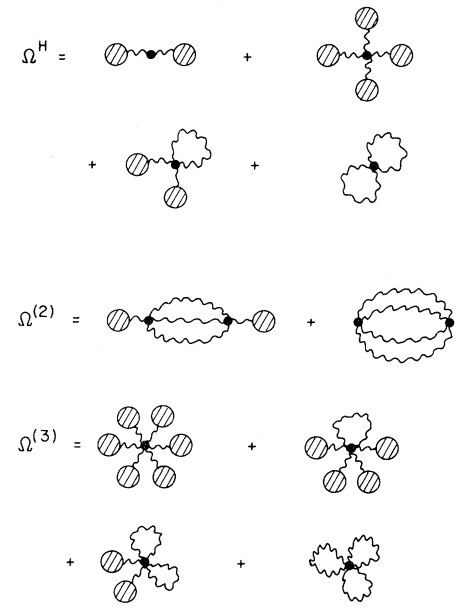

FIG. 2. The Φ-diagrams from which various approximations in the text are derived. The wavy line is $\tilde{D}_q$ in (3.15); the terminated line is D in Eq. (3.13). The Ω^H generates the Hartree approximation in the text; $\Omega^{(2)}$ corresponds to the Born approximation; $\Omega^{(3)}$ is the Hartree approximation for a three-body term.

A. Series for the thermodynamic potential

As mentioned before, the exact perturbation series for the thermodynamic potential W considered as a functional of D and $\tilde{D}_q$ satisfies the stationary properties $\delta W / \delta D = 0$ and $\delta W / \delta \tilde{D}_q = 0$. In order to use the stationary conditions an explicit representation of W in terms of D and $\tilde{D}_q$ is needed. Obtaining this representation is problematic because of the well-known counting difficulty from factors of n^{-1} in closed loop diagrams with n-fold symmetry, but it nevertheless has been worked out by Luttinger and Ward[17] for the nonanomalous case and De Dominicus and Martin[15] in general.

The expression for W is found to have the form

$$W = -\tfrac{1}{2} D^2 + \tilde{H} D - \frac{1}{2N} \sum_q \left(\ln \tilde{D}_q^{-1} + \Sigma_q \tilde{D}_q \right) + \Omega' , \tag{4.2}$$

where Ω' is the set of irreducible diagrams for W, but with the full D and $\tilde{D}_q$ substituted for bare lines. Here Σ_q is the self-energy, defined as $\tilde{D}_q \equiv (1 - \Sigma_q)^{-1}$.

The diagrams for Ω' corresponding to the Hartree approximation are given by Ω^H in Fig. 2. Molecular field theory to third order in the magnetization is given by the first two diagrams; the next two represent the effect of fluctuations.

We investigate the following corrections to the Hartree approximation: the second-order (Born-approximation) diagrams in β_F are given by $\Omega^{(2)}$ in Fig. 2; the first-order diagrams in κ_F (the three-body interaction) are given by $\Omega^{(3)}$ in Fig. 2. In addition we estimate the effect of the weak temperature dependence of α_F given in Eq. (2.11).

We shall identify the corrections below by superscripts pertaining to the Ω' diagrams from which they are derived. From functionally differentiating Ω^H, $\Omega^{(2)}$, and $\Omega^{(3)}$, respectively, we find $\delta W/\delta D = 0$ can be rewritten $D = D^H + D^{(2)} + D^{(3)}$, where

$$D^H = \tilde{H} - (\alpha_F - 1)D - (\beta_F \tilde{T}/3!N)D^3 - \tfrac{1}{2}\beta_F \tilde{T} D\xi, \tag{4.3a}$$

$$D^{(2)} = [(\beta_F \tilde{T})^2/3!]\, g_1(\eta; 0)\, D, \tag{4.3b}$$

$$D^{(3)} = -\kappa_F \tilde{T}^2 \left(\frac{D^2}{5!N^2} + \frac{\xi^2 D}{8} + \frac{\xi D^3}{24N} \right), \tag{4.3c}$$

and

$$g_1(\eta; q) = N^{-2} \sum_{q'q''} \tilde{D}_{q'} \tilde{D}_{q''} \tilde{D}_{q+q'+q''}.$$

Unless there is no chance of confusion, in the following, quantities defined in the Hartree approximation will be denoted by a superscript H, whereas fully renormalized quantities will bear no superscript.

To find $\tilde{D}_q$ we use the stationary property $\delta W/\delta \tilde{D}_q = 0$, which reduces to equations for the self-energy $\Sigma = \Sigma^H + \Sigma^{(2)} + \Sigma^{(3)}$, if we note the stationary property requires $\delta\Omega'/\delta D_q \equiv \tfrac{1}{2}\Sigma_q$. We obtain

$$\Sigma^H = -(\alpha_F - 1 + \mu_F^2 q^2) - \frac{\beta_F \tilde{T}\xi}{2} - \frac{\beta_F \tilde{T}}{2!N} D^2, \tag{4.4a}$$

$$\Sigma^{(2)} = \frac{(\beta_F T)^2}{2N} D^2\, g_2(\eta; q) + \frac{(\beta_F \tilde{T})^2}{3!} g_1(\eta; q), \tag{4.4b}$$

$$\Sigma^{(3)} = -\kappa_F \tilde{T}^2 \left(\frac{\xi^2}{8} + \frac{\xi D^2}{4N} + \frac{D^4}{4!N^2} \right), \tag{4.4c}$$

where

$$g_2(\eta; q) = N^{-1} \sum_{q'} \tilde{D}_{q+q'} \tilde{D}_{q'}.$$

To obtain proper expansions in ϵ and $\tilde{T}$, the $\Omega^{(2)}$ and $\Omega^{(3)}$ corrections must be incorporated self-consistently in the definition of ξ and D on the right-hand sides of (4.3a) and (4.4a). However, to the order to which we are interested, Hartree expressions for $\tilde{D}_q$ and D can be used in the $\Omega^{(2)}$ and $\Omega^{(3)}$ contributions themselves. We neglect the momentum dependence of the $\Omega^{(2)}$ corrections in the following.

B. Magnetization

The equation for the magnetization can be obtained by rearranging (4.3):

$$y = -(\alpha_F + \tfrac{1}{2}\beta_F \tilde{T}\xi) + x + [D^{(2)} + D^{(3)}]D^{-1}, \tag{4.5}$$

where

$$y = \beta_F \tilde{T} D^2/3!N = \tfrac{1}{12}\beta_F (\Delta n + H')^2, \quad x = \tilde{H}/D = H'/(\Delta n + H'). \tag{4.6}$$

These latter results follow from $\tilde{T} \equiv T/2U$, $\tilde{H} \equiv \mu_B H (N/UT)^{1/2}$, and (3.13) with $H' = \mu_B H/U$. Here Δn is the difference in the spin-up and spin-down electrons per site. Generally, $H' \ll \Delta n$ and y and x are then the usual Arrott[18] plot variables.

We shall discuss only the behavior in weak fields in the presence of the higher-order corrections. Generally, these affect the magnetization not only through the explicit $D^{(2)}$ and $D^{(3)}$ terms in (4.5) but also through self-consistent renormalization of ξ. These effects are found to be comparable.

1. $T < T_C$

The weak-field limit for $T < T_C$ can be taken to be $x \ll |\eta_0|$. We first obtain the general expression for η from (4.3) and (4.4):

$$\eta = -2(\alpha_F + \tfrac{1}{2}\beta_F \tilde{T}\xi) + |\eta_0|\lambda, \tag{4.7}$$

where $\lambda = 3x/|\eta_0| + \lambda^{(2)} + \lambda^{(3)}$ and

$$|\eta_0|\lambda^{(2)} = \tfrac{1}{3}(\beta_F \tilde{T})^2 g_1(\eta; 0) - 3\beta_F \tilde{T} g_2(\eta; 0)y, \quad |\eta_0|\lambda^{(3)} = -\tfrac{1}{4}\kappa_F \tilde{T}^2 \xi^2 + 3\kappa_F y^2/5\beta_F^2. \tag{4.8}$$

In the following, the momentum dependence at finite q of $\lambda^{(2)}$ will be neglected. In this case the self-consistency Eq. (3.9) is modified only by a "shift" in T_C; one replaces η_0 by $\eta_0(1 + \tfrac{1}{2}\lambda)$ in (3.9). Again approximating the arctangent[14] by $\tfrac{1}{2}\pi$, we obtain the expansion

$$\eta = 2|\eta_0|(1 + \tfrac{1}{2}\lambda)(1 + \epsilon'^{1/2} + \tfrac{1}{2}\epsilon' + \tfrac{1}{8}\epsilon'^{3/2} + \cdots), \tag{4.9}$$

where $\epsilon' = \epsilon[2(1 + \tfrac{1}{2}\lambda)]^{-1}$.

Leading $q = 0$ terms from integrals in $\lambda^{(2)}$, sufficient for our purposes, are easily evaluated:

$$[(\beta_F \tilde{T})^2/3!]\, g_1(\eta; 0) \approx \gamma_F^2 \tilde{T}^2 \ln(\mu_F^2 q_m^2/\eta), \quad \beta_F \tilde{T} g_2(\eta; 0) = \gamma_F \tilde{T} \eta^{-1/2}. \tag{4.10}$$

Had we kept the momentum dependence of $\lambda^{(2)}$, we would have found only that the right-hand side of (4.10), which falls off with q, overestimates slightly the importance of these correction terms.

We also note that $[D^{(2)} + D^{(3)}]D^{-1}$ can be written

$$[D^{(2)} + D^{(3)}]D^{-1} = (\beta_F \tilde{T})^2 g_1(\eta; 0)/3! - \kappa_F (3!)^2 y^2/5!\beta_F^2 - \kappa_F \tilde{T}^2 \xi^2/8 - \kappa_F \tilde{T}\xi y/2\beta_F. \tag{4.14}$$

Finally we need to start collecting expressions. Equations (4.9) and (4.7) define $\alpha_F + \tfrac{1}{2}\beta_F \tilde{T}\xi$, which can be substituted into (4.5). It is sufficient, to leading order in all corrections, to use

$$y = x + |\eta_0| \left(1 + \frac{\epsilon^{1/2}}{(2)^{1/2}} (1 + \tfrac{1}{4}\lambda - \tfrac{1}{32}\lambda^2) \right.$$

$$+\frac{\epsilon}{4}+\frac{\epsilon^{3/2}\lambda}{64(2)^{1/2}}\Big)+[D^{(2)}+D^{(3)}]D^{-1}.$$

We can also set $y\simeq|\eta_0|+x$ and $\eta\simeq 2|\eta_0|+3x$, where these appear in λ and $[D^{(2)}+D^{(3)}]D^{-1}$.

For $x\ll|\eta_0|$ it is straightforward, if a bit tedious, to derive from (4.8), (4.10), and (4.11) the result

$$y=y_0+y_1, \tag{4.12a}$$

where

$$y_0=|\eta_0|\,[1+\epsilon^{1/2}/(2)^{1/2}+\text{C.T.}], \tag{4.12b}$$

$$y_1=x\left(1+\frac{3\epsilon^{1/2}}{4(2)^{1/2}}-\frac{9\epsilon^{1/2}}{32(2)^{1/2}}\frac{x}{|\eta_0|}+\text{C.T.}\right) \tag{4.12c}$$

with correction terms specified in Table I. Here, x and y are the Arrott plot variables in Eq. (4.6). It is easy to generalize λ to include the temperature dependence (2.11) for α_F and this result is indicated in the caption of Table I. In order to reduce the complexity of the entries the order of magnitude of the various small parameters has been ranked according to $\eta_0\ll\beta_F\tilde{T}\xi_0$. In addition, terms of order $\epsilon^{3/2}$ have been neglected compared to $\tilde{T}$ and ϵ.

Equation (4.12) gives the order of magnitude of curvature effects in the Arrott plot of y vs x for *weak* fields.[19] The spacing of isotherms is not simply proportional to $|\eta_0|\propto(T-T_C)$ but is also affected by $\epsilon^{1/2}$ corrections in the Hartree approximation and corrections of order $\epsilon\ln(\Delta T/T_0)$ from $\Omega^{(2)}$. These could be comparable. The curvature of the isotherms from the $\epsilon^{1/2}x^2/|\eta_0|$ dependence in (4.12), however, dominates contributions of order $\epsilon x^2/|\eta_0|$ from $\Omega^{(2)}$ which have therefore been dropped from Table I.

The singular part of the susceptibility is also given by (3.14) as

$$\chi_s=\mu_B^2/\eta U$$

We obtain, from (4.7)–(4.9), the result in zero field

$$\chi_s=\mu_B^2[2U|\eta_0|(1+\text{C.T.})]^{-1}. \tag{4.13}$$

For $T<T_C$, the $\epsilon^{1/2}$ Hartree contribution is comparable to that from $\Omega^{(2)}$ and so has been entered in Table I.

2. $T>T_C$

For $T>T_C$, the small quantity in weak fields is y, not x, which is comparable to η_0. We substitute for x, from (4.5), into (4.7) to obtain

$$\eta=\alpha_F+\tfrac{1}{2}\beta_F\tilde{T}\xi+\eta_0\tilde{\lambda}, \tag{4.14}$$

where the small quantity $\eta_0\tilde{\lambda}$ is given by

$$\eta_0\tilde{\lambda}=3y+\eta_0\tilde{\lambda}^{(2)}+\eta_0\tilde{\lambda}^{(3)},$$

where

$$\eta_0\tilde{\lambda}^{(2)}=-\tfrac{1}{2}3!\,\beta_F\tilde{T}yg_2(\eta;0)-(\beta_F\tilde{T})^2g_1(\eta;0)/3!\,,$$

$$\eta_0\tilde{\lambda}^{(3)}=\kappa_F\tilde{T}^2(\tfrac{1}{8}\xi^2+D^4/4!+\tfrac{1}{4}\xi D^2)\,.$$

Again the correction can be treated as a shift in T_C. From (3.11), we obtain

$$\eta\simeq\eta_0(1+\tilde{\lambda})(1-\tilde{\epsilon}^{1/2}+\tfrac{1}{2}\tilde{\epsilon}-\cdots), \tag{4.15}$$

where $\tilde{\epsilon}=\epsilon/(1+\tilde{\lambda})$.

To derive the leading corrections to the magnetization equation, it is sufficient to consider, from (4.5), (4.14), and (4.15)

$$y=x-\eta_0[1-\epsilon^{1/2}(1+\tfrac{1}{2}\tilde{\lambda}-\cdots)+\tfrac{1}{2}\epsilon+3\epsilon^{3/2}y/16+\cdots]$$
$$+(D^{(2)}+D^{(3)})D^{-1}, \tag{4.16}$$

where $\tilde{\lambda}$, $D^{(2)}$, and $D^{(3)}$ are evaluated using $\eta\simeq\eta_0+3y$. From (4.10), (4.11), and (4.14) we obtain, for $y\ll\eta_0\ll1$, $\epsilon\ll1$,

$$x=x_0+x_1, \tag{4.17a}$$

$$x_0=\eta_0(1-\epsilon^{1/2}+\text{C.T.}), \tag{4.17b}$$

$$x_1=y[1-\tfrac{3}{2}\epsilon^{1/2}(1-3y/4\eta_0)+\text{C.T.}], \tag{4.17c}$$

where x and y are again the Arrott variables in (4.6).

In zero field, y vanishes and one easily obtains the correction terms for the zero-field susceptibility (3.16) from (4.14).

C. Specific heat in zero field

We again use Eq. (3.5), where W is given by Eq. (4.2). The first derivative of dW/dT is easy because the temperature dependence of D and $\tilde{D}_q$ does not contribute, because of the stationary properties. The explicit temperature dependence of the various interactions and that of the explicit upper limit q_m in diagrams is all that need be taken into account. Let us examine the latter dependence in more detail. What essentially happened in dW/dT in the Hartree approximation in (3.1) was that the derivative of the upper limit of the fourth $\int dq\Sigma_qD_q$ term in (4.2) cancelled against the derivative of the upper limits of the product of Hartree integrals in the last contribution for Ω^H in Fig. 2. Thus dW/dT had no term like $d\xi/dT$. Analysis of diagram symmetry factors suggests this always happens as long as only Hartree loops are present, as in Ω^H and $\Omega^{(3)}$. In the $\Omega^{(2)}$ diagrams cancellation does *not* occur, although it is not entirely clear whether q_m should be used in these integrals. However, including the temperature dependence of q_m or not in these corrections makes a difference only between T^2 or $T^2\ln q_m\sim T^2\ln T$ in the first $\Omega^{(2)}$ diagram of Fig. 2 and T^2 or $T^2q_m\sim T^{7/3}$ in the second. We thus ignore q_m temperature dependence in $\Omega^{(2)}$.

We are then left with the upper limit of the $\ln D_q$ integral in (4.2). Differentiation of this limit gives rise to the same background contribution C_b/T in

Eq. (3.8) for $T< T_C$ as $T>T_C$, since the only change is that $D_{q_m}\approx(2|\eta_0|+\mu_F^2q_m^2)$ for $T<T_C$ instead of $D_{q_m}\approx(\eta_0+\mu_F^2q_m^2)$ for $T>T_C$ and the $|\eta_0|$ is negligible anyway in the limit (3.7).

Continuing on to evaluate $\Delta C_{\rm crit}/T$, we differentiate the explicit temperature dependence of $v_2=\beta_F\tilde{T}$ (the vertex with four lines) in the Hartree contribution Ω^H in Fig. 2:

$$\begin{aligned}\frac{d\Omega^H}{dT}&=\frac{-\beta_F}{4U}\left(\tfrac{1}{4}\xi D^2+N\xi^2+D^4/4!N\right)\\&=-\beta_F\xi^2/16U\quad T>T_C\\&=+\beta_F\xi^2/8U-3\alpha_F^2\left(4U\tilde{T}^2\beta_F\right)^{-1}\\&\quad+\frac{3\beta_F}{2UD}\left(D^{(2)}+D^{(3)}\right)\left(\alpha_F-\frac{\left(D^{(2)}+D^{(3)}\right)}{2\beta_F^2\tilde{T}^2D}\right),\quad T<T_C,\end{aligned}\tag{4.18}$$

where the last line is obtained from (4.5). The last term for $T<T_C$ involving $(D^{(2)}+D^{(3)})^2$ does not contain important corrections and will be neglected.

In order to calculate C/T, the explicit form for ξ can be obtained from (4.14) and (4.15) for $T>T_C$ and (4.7) and (4.9) for $T<T_C$. The self-consistent renormalization effects can be included by retaining terms first power in $\tilde{\lambda}$ and λ, respectively, in the iteration for ξ. From (3.5) and (4.18), we see that the specific heat will have a contribution proportional to

$$\xi(\xi+\tilde{T}\,d\xi/d\tilde{T}).$$

Effects from the $\Omega^{(2)}$ and $\Omega^{(3)}$ diagrams in Fig. 2 are generally comparable to those from the self-consistent renormalization of ξ. These are evaluated in a straightforward fashion from (3.5) using the Hartree expressions for η and y. For completeness, we give the first derivatives (ignoring the temperature dependence of q_m for reasons above):

$$\begin{aligned}\frac{d\Omega^{(2)}}{dT}&=\frac{\beta_F^2\tilde{T}Ng_3(\eta)}{48U}+\frac{\beta_F yNg_1(\eta;\,0)}{2U},\\\frac{d\Omega^{(3)}}{dT}&=-\frac{\kappa_F\tilde{T}N}{U}\left(\frac{\xi^3}{48}+\frac{3\xi y^2}{4\beta_F^2\tilde{T}^2}+\frac{3\xi^2y}{8\beta_F\tilde{T}}+\frac{3}{10}\frac{y^3}{(\beta_F\tilde{T})^3}\right),\end{aligned}\tag{4.19}$$

where

$$g_3(\eta)=N^{-3}\sum_{qq'q''}\tilde{D}_q\tilde{D}_{q'}\tilde{D}_{q''}\tilde{D}_{q+q'+q''}.$$

The approximation used for g_3 is $g_3(\eta)\simeq g_3(0)=\frac{1}{32}\xi_0^3\pi^2\kappa/\mu_F^2q_m^2$, where κ is a constant of order unity. Also, if the temperature dependence (2.11) of α_F is taken into account, we must include derivatives of diagrams first order in v_1:

$$\left.\frac{dW}{dT}\right|_{v_1}=-\left(\frac{3y}{\beta_F\tilde{T}}-\xi\right)N\frac{d}{dT}\alpha_F,\tag{4.20}$$

in addition to including $\Delta\alpha_F$ in the definition of λ and $\tilde{\lambda}$.

Carrying out the indicated algebra, one obtains (3.12) plus corrections at $T>T_C$ and

$$C/T=\Delta C_{\rm crit}/T+C_b/T,$$

where

$$\frac{\Delta C_{\rm crit}}{T}=\frac{\beta_F\xi_0^2}{4U}\left(1+\frac{Td\ln q_m}{dT}+\frac{(2)^{1/2}}{4}\epsilon^{1/2}-\frac{(2)^{1/2}}{4}\pi\left(\frac{\Delta T}{T_0}\right)^{1/2}+\text{C.T.}\right)\tag{4.21}$$

for $T<T_C$. Again the various correction terms are tabulated in Table I. According to the above discussion, C_b/T is given by Eq. (3.8) for $T>T_C$ or $T<T_C$, provided (3.7) holds.

D. Difficulty in thermodynamic consistency for $T<T_C$

We discuss the interesting difficulty that our variationally derived expression for the susceptibility for $T<T_C$ is not thermodynamically consistent. The inconsistency is small for small ϵ but not otherwise.

The difficulty is that separate approximations are made for the order parameter D and the mean-squared fluctuation amplitude $\tilde{D}_q$; that is, the free energy W is considered a functional of D and $\tilde{D}_q$ separately, which are then defined from stationary conditions. The problem is that D and $\tilde{D}_q$ then do not necessarily satisfy the relation obtained through Eqs. (3.13) and (3.14):

$$\chi=\frac{\mu_B^2}{U}\frac{d(D-\tilde{H})}{d\tilde{H}}=\frac{\mu_B^2}{U}(\tilde{D}_{q=0}-1).\tag{4.22}$$

We shall take the Hartree approximation as an example. The magnetization is given by Eq. (4.5) with $D^{(2)}$ and $D^{(3)}$ set to zero. The fluctuation amplitude $\tilde{D}_{q=0}\equiv\eta$ is given by Eq. (4.7). These expressions are variationally derived from Ω^H in Fig. 2. If we calculate the susceptibility by differentiating the order parameter, we obtain

$$\frac{dD}{d\tilde{H}}=\left(1-\tfrac{1}{2}\beta_F\tilde{T}D\frac{d\xi}{d\tilde{H}}\right)\left[-2\left(\alpha_F+\tfrac{1}{2}\beta_F\tilde{T}\xi\right)+3\tilde{H}/D\right]^{-1},\tag{4.23}$$

where all quantities are defined in the Hartree approximation. This, when substituted into (4.22), gives a result different from that from substitution of $D_{q=0}\equiv\eta$ and (4.7) into (4.22). The difficulty is that the field dependence of ξ generates an infinite heirarchy of self-energy corrections, which would have to put into $\tilde{D}_q$, to make the two expressions agree.

To see this, from (4.5) (with $D^{(2)}=D^{(3)}=0$), (4.6), and (4.7), we first write $\tilde{D}_q$ as

$$\tilde{D}_q=\left[\alpha_F+\tfrac{1}{2}\beta\tilde{T}\xi+(\beta_FT)^2D^2/2N\right]^{-1}.\tag{4.24}$$

By definition, we obtain

$$\frac{d\xi}{d\tilde{H}}=-\frac{1}{N}\sum_q\tilde{D}_q^2\left(\frac{\beta_F\tilde{T}}{2}\frac{d\xi}{d\tilde{H}}+\frac{\beta_F^2\tilde{T}D}{N}\frac{dD}{d\tilde{H}}\right).\tag{4.25}$$

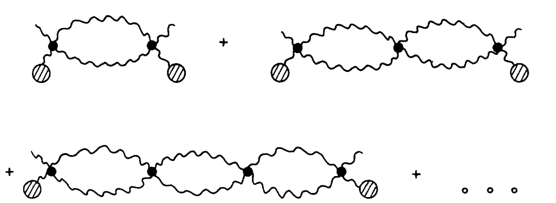

FIG. 3. The self-energy series required for a completely thermodynamically consistent (gapless) theory for finite magnetization.

By solving (4.25) for $d\xi/d\tilde{H}$ and substituting into (4.23), we obtain

$$\frac{dD}{d\tilde{H}}=\tilde{D}_q^{-1}-\frac{(\beta_F\tilde{T})^2D^2g_2(\eta;\,0)}{2N[1+\frac{1}{2}\beta_F\tilde{T}g_1(\eta;0)]}\quad, \tag{4.26}$$

where g_2 is the integral given after Eq. (4.4).

Therefore, the susceptibility in Eq. (4.22) would have to be defined with the additional self-energy

$$\Sigma'=\frac{(\beta_F\tilde{T})^2D^2g_2(\eta;\,0)}{2N[1+\frac{1}{2}\beta_F\tilde{T}g_2(\eta;\,0)]} \tag{4.27}$$

to make the thermodynamics consistent. This self-energy is generated by differentiating the field dependence of ξ in the magnetization equation and corresponds to the infinite set of diagrams given in Fig. 3. (We note in this figure and in g_2 in (4.27) that for full thermodynamic consistency—i.e., satisfaction of (4.22)—the propagators should be the Hartree ones (4.24) rather than the ones fully renormalized with Σ' itself.)

The first of these self-energy diagrams in the approximation that Hartree propagators are used for for the internal lines is what we evaluated for the first term of $\Sigma^{(2)}$ in (4.4b). The effect of this contribution on the thermodynamics for $T<T_C$ is essentially given by the nonlogarithmic entries under $\Omega^{(2)}$ in Table I. Thermodynamic consistency thus fails at order ϵ or $\epsilon^{1/2}$, depending on the property considered. This difficulty is reminiscent of the notorious discrepancy between gapless and conserved approximations in superfluid boson systems.[20]

V. INFLUENCE OF LOWEST-ORDER DYNAMIC CORRECTIONS

The motivation for the classical description (2.1) of the phase transition is that longer and longer wavelength fluctuations become important as one approaches T_C. When these fluctuations begin to involve macroscopic regions, one ought to be able, in some sense, to neglect finite-frequency modes, which are necessitated by noncommutivity of operators in the first place.[21] However, simply neglecting the finite-frequency modes is somewhat simplistic. Although the form (2.1) is valid in the phase-transition region, the finite-frequency modes still determine the coefficients α_F and β_F and the cutoff q_m to be used in the model. We shall see next how this can occur.

Whereas in the classical model the properties of electrons were contained in the structureless coefficients α_F and β_F, the dynamics of the electrons now need to be made explicit. The propagator $D_{qn}=\langle h_{qn}h_{qn}^*\rangle=(1-\Sigma_{qn})^{-1}$, defined in terms of the generalized ensemble average, depends on the thermal frequency $\omega_n=2\pi inT$ through the self-energy, taken to be

$$\Sigma_{qn}=2U\Phi_{qn}^{(2)}-\tfrac{1}{2}\beta_F^0\tilde{T}\xi-\alpha^{(1)}, \tag{5.1}$$

where $\Phi_{qn}^{(2)}$ is given in (A4). To insure stability we have included the effect of coupling of the static modes to lowest order through the β_F term, and in $\alpha^{(1)}$ we have allowed for self-consistent renormalization effects of finite-frequency modes. The effective mode number ξ is defined as in (3.3) as a sum over q for $q<q_m$ of $\tilde{D}_{q,n=0}$. The cutoff q_m should not be confused with the cutoff $q_m'=O(k_F)$ below, determined from the lattice spacing. The parameter q_m at this point is basically at our disposal and will be chosen to make the thermodynamic behavior particularly simple. It is chosen to appear only as an effective momentum cutoff in the dynamically renormalized susceptibility, so that direct correspondence can be made with the cutoff in the model (2.1). For *weak* transitions, a direct identification of the GL coefficients can also be made from the expansions of the renormalized susceptibility in powers of fluctuations.

We define α_F^0 as in (2.10) to be the contribution to $1-\Sigma_{q=0,n=0}$, which is explicitly zero order in the static and finite-frequency modes. The lowest-order renormalization from the finite-frequency modes is given by the three diagrams of Fig. 4 for $\alpha^{(1)}$.

The contribution to $\alpha_F^{(1)}$ from the first diagram is given by

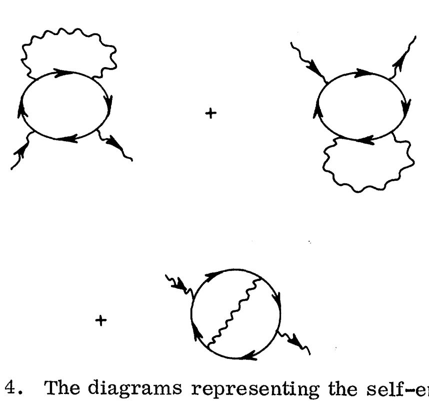

FIG. 4. The diagrams representing the self-energy to first order in the finite-frequency fluctuations. The solid lines are electrons.

$$\frac{2U^2T^2}{N^2}\sum_{\substack{kq\\n,m}}{}^{\prime}\,\tilde{D}_{qm}G_{k-q,n-m}G^3_{kn}\,. \qquad (5.2)$$

The prime convention implies that for $m=0$, only modes with $q>q_m$ are to be included.

We first write

$$T\sum_{\substack{q\\m\neq 0}} D_{qm}G_{k-q,n-m}=\frac{1}{2\pi i}\oint\frac{dz[n(z)+\frac{1}{2}]D_q(z)}{\omega_n-z-\epsilon_{k-q}}\,, \qquad (5.3)$$

where the contour encloses the poles of $n(z)=(e^{z/T}-1)^{-1}$ and that of $(\omega_n-z-\epsilon_{k-q})^{-1}$. So, Eq. (5.3) becomes

$$-T\sum_q^{q_m} D_q(0)\,G_{k-q}(\omega_n)+\frac{1}{\pi}\sum_q^{q'_m}\oint\frac{d\omega'[n(\omega')+\frac{1}{2}]\,\mathrm{Im}\tilde{D}_q(\omega'+i\delta)}{\omega_n-\omega'-\epsilon_{k-q}}-\sum_q^{q'_m}[f(-\epsilon_{k-q})-\tfrac{1}{2}]\tilde{D}_q(\omega_n-\epsilon_{k-q})\,, \qquad (5.4)$$

where f is the Fermi function and the ω' contour encloses the real axis.

We discuss the term involving the Fermi factor first. The comparable term for the electron self-energy in paramagnon theory leads to large effective-mass corrections in the specific heat away from the phase transition.[2] The contribution to α_F, however, is not particularly important.

The Fermi terms from the three diagrams of Fig. 4 yield

$$\alpha^{(1)}_{\mathrm{fermion}}=\frac{2U^2}{2\pi iN}\sum_{k,q}\oint dz\bigg(\frac{2[f(z)-\frac{1}{2}][f(-\epsilon_{k-q})-\frac{1}{2}]}{(z-\epsilon_k)^3}\times\tilde{D}_q(z-\epsilon_{k-q})-\frac{f(z)-\frac{1}{2}}{(z-\epsilon_k)^2}\frac{\partial}{\partial\epsilon_{k-q}}\times\{[f(-\epsilon_{k-q})-\tfrac{1}{2}]\tilde{D}_q(z-\epsilon_{k-q})\}\bigg)\,. \qquad (5.5)$$

If we assume that $\epsilon_k\simeq 0$ and $q\lesssim k_F$ are the important integration regions, then we can approximate $\epsilon_{k-q}\simeq\epsilon_k-\vec{q}\cdot\vec{V}_F$. In that case one can do the ϵ_k integral by parts and take advantage of a partial Ward-identity cancellation between the first and second terms of (5.5):

$$\alpha^{(1)}_{\mathrm{fermion}}=\frac{2U^2}{2\pi iN}\sum_q\oint dz\int d\epsilon\,\frac{d\Omega}{4\pi}N'(\epsilon)[f(z)-\tfrac{1}{2}]\times\frac{[f(-\epsilon_k+q-V_F)-\frac{1}{2}]\tilde{D}_q(z-\epsilon_k+\vec{q}\cdot\vec{V}_F)}{(z-\epsilon_k)^2}\,. \qquad (5.6)$$

The symmetry of the integrand in (5.5) under change of sign of z, ϵ, and $\vec{q}\cdot\vec{V}_F=qV_F\cos\theta$ and use of $\tilde{D}_q(\omega+i\delta)=\tilde{D}_{-q}(-\omega-i\delta)$ from (5.1) implies that only the odd part of $N'(\epsilon)$ contributes. Therefore, in (5.6) we can keep only the *second* term in the expansion of

$$N'(\epsilon)\approx N'(\epsilon_F)+(\epsilon-\epsilon_F)N''(\epsilon_F)\,. \qquad (5.7)$$

We argue that important temperature dependence is not generated by the explicit Fermi factors in (5.5). The argument is given as follows: The derivative of a Fermi factor is a representation for the derivative of a δ function with weight proportional to T:

$$\frac{d}{dT}f(\epsilon)\approx-\frac{\pi^3T}{2}\,\delta'(\epsilon)\,. \qquad (5.8)$$

Therefore, if the explicit Fermi factors in (5.6) are differentiated, the contribution to $d\alpha^{(1)}_{\mathrm{fermion}}/dT$, is of order T/ϵ_F, from dimensional arguments, *provided the integrals after* (5.8) *is used are nonsingular at* $T=0$. If the remaining integrals are singular, a factor of T^{-1} can of course be generated at finite temperature which cancels the factor of T in (5.8).

We have examined the nature of the singularities in the terms of $d\alpha^{(1)}_{\mathrm{fermion}}/dT$ arising from differentiating the Fermi factors in (5.6). We use the explicit, standard paramagnon form for $\tilde{D}_q$ derived from evaluating $\Phi^{(2)}(q,\omega\pm i\delta)$:

$$\tilde{D}_q(\omega\pm i\delta)=(\eta+\mu_F^2q^2\mp i\omega/\gamma q)\,, \qquad (5.9)$$

where

$$\eta=\alpha^0_F+\alpha^{(1)}+\tfrac{1}{2}\beta^0_F\tilde{T}\xi \qquad (5.10)$$

and $\gamma=2V_F[2UN(\epsilon_F)\pi]^{-1}$. (This expression is valid for $\omega\leq V_Fq$. For $\omega\geq V_Fq$ we note that $\tilde{D}_q(\omega)$ is strictly real.) Using (5.7), (5.8), and (5.9) and introducing the temperature as a cutoff, we find from detailed examination that the contribution from these terms is at most of order $(T/\epsilon_F)\times\ln(T/\epsilon_F)$. Therefore, the Fermi factors in (5.6) contribute temperature dependence at most of order $(T/\epsilon_F)^2\ln(T/\epsilon_F)$ to $\alpha^{(1)}_{\mathrm{fermion}}$. This result depends heavily on the partial Ward-identify cancellation, which, along with the second term of (5.7) reduces the singularity of the integrand in (5.6).

The important contribution to $d\alpha^{(1)}_{\mathrm{fermion}}/dT$ will be seen to arise from differentiating the temperature dependence of η in Eq. (5.9), which is bootstrapped by the β^0_F term in (5.1). From the spectral representation of $\tilde{D}_q$ and use of the explicit form (5.9), we obtain

$$\frac{d\alpha^{(1)}_{\mathrm{fermion}}}{dT}=-\frac{2U^2}{2\pi^2N}\frac{d\eta}{dT}\sum_q\gamma q\int d\omega\,d\omega'\,d\epsilon N'(\epsilon)$$

$$\times 2\mathrm{Im}\int_{-qV_F}^{qV_F} \frac{dy}{2qV_F} \frac{[f(\omega)-\frac{1}{2}][f(-\epsilon+y)-\frac{1}{2}]}{(\omega-\epsilon+i\delta)^2(\omega-\epsilon+y-\omega'+i\delta)} \frac{\partial}{\partial\omega'}\mathrm{Re}\tilde{D}_q(\omega')+O\left(\frac{T}{\epsilon_F}\ln\left(\frac{T}{\epsilon_F}\right)\right) .$$

The ω integration is easily done. Using the fact that $\mathrm{Re}\tilde{D}_q(\omega')$ is sharply peaked around $\omega'\sim\Gamma(q)\equiv\gamma_q(\eta+\mu_F^2q^2)\ll V_Fq$, one can do the ω' integral by parts. Using the Lorentzian approximation for $\mathrm{Re}\tilde{D}_q(\omega')$ and (5.7), we finally obtain

$$\frac{d\alpha^{(1)}_{\text{fermion}}}{dT}=\frac{U^2\Omega_qN''(\epsilon_F)\gamma^2}{2\pi^2V_FN}\int_0^{q'_m} q^3dq\ln\left(\frac{qV_F}{\Gamma(q)}\right)\frac{d\eta}{dT}+O\left(\frac{T}{\epsilon_F}\ln\left(\frac{T}{\epsilon_F}\right)\right). \tag{5.11}$$

The fact that the coefficient of $d\eta/dT$ is of order 1 implies that β_F^0 will be renormalized in (5.1). Before discussing this result, however, let us go back to examine the remaining contribution to $\alpha^{(1)}$.

The remaining boson contribution to $\alpha^{(1)}$ from (5.4) can be rewritten by using the fact that the single pole approximation for $n(\omega')$ corresponds to keeping the $m=0$ term in the sum over m. For the three diagrams in the scalar theory, we have

$$\alpha^{(1)}_{\text{boson}}=-\frac{2U^2}{2\pi^2iN^2}\sum_{qk}{}'\int d\omega'\int d\omega\left(n(\omega')-\frac{T}{\omega'}+\frac{1}{2}\right)\mathrm{Im}\tilde{D}_q(\omega'+i\delta)[f(\omega)-\tfrac{1}{2}]\times\left(\frac{2}{(\omega-\omega'-\epsilon_{k-q})(\omega-\epsilon_k)^3}+\frac{1}{(\omega-\omega'-\epsilon_{k-q})^2(\omega-\epsilon_k)^2}\right), \tag{5.12}$$

where the primed summation indicates that q is restricted to $q<q_m$ in the term involving T/ω'. Now, $\mathrm{Im}\tilde{D}_q(\omega'+i\delta)$ vanishes for $|\omega'|>V_Fq$. In this case the structure imposed by the ω' and q dependence in the denominators of (5.12) can be neglected. Doing the ω integration, we obtain

$$\alpha^{(1)}_{\text{boson}}=-\frac{U^2N''(\epsilon_F)}{\pi N}\sum_q{}'\int d\omega'\left(n(\omega')-\frac{T}{\omega'}+\frac{1}{2}\right)\times\mathrm{Im}\tilde{D}_q(\omega'+i\delta). \tag{5.13}$$

We will calculate next the temperature dependence of $\alpha^{(1)}_{\text{boson}}$ due only to the η dependence of $\mathrm{Im}\tilde{D}_q(\omega+i\delta)$ in (5.13). We define q_m so that it exactly compensates the temperature dependence of the statistical factor in large parentheses in (5.13). In the renormalized susceptibility, this results in q_m appearing only as a cutoff in momentum integrals, which is what is desired to make contact with the cutoff in the model (2.1).

We first add and subtract the region $q_m<q<q'_m$ in the momentum sum for the T/ω term, and then use $\pi^{-1}\int\mathrm{Im}\tilde{D}_q(\omega')=\mathrm{Re}\tilde{D}_q(0)$.

$$\alpha^{(1)}_{\text{boson}}=-\frac{U^2N''(\epsilon_F)}{N}\left[\frac{1}{\pi}\sum_q^{q'_m}\int d\omega'\left(n(\omega')-\frac{T}{\omega'}-\frac{1}{2}\right)\times\mathrm{Im}\tilde{D}_q(\omega')+T\sum_{q=q_m}^{q'_m}\mathrm{Re}\tilde{D}_q(0)\right]. \tag{5.14}$$

Next we write

$$\mathrm{Im}D_q(\omega+i\delta)=\frac{\gamma q}{2}\frac{\partial}{\partial\omega}\ln[\Gamma^2(q)+\omega^2],$$

where $\Gamma(q)=\gamma q(\eta+\mu_F^2q^2)$. One can do the ω' integration by parts, and neglect endpoint corrections so far as the temperature dependence of $\alpha^{(1)}_{\text{boson}}$ is concerned. Using the fact that $\partial[n(\omega)-T/\omega-\frac{1}{2}]/\partial\omega$ is sharply peaked with weight unity, we obtain

$$\alpha^{(1)}_{\text{boson}}=\frac{U^2N''(\epsilon_F)}{N}\left(\frac{1}{2\pi}\sum_q^{q'_m}\gamma q\ln\Gamma^2(q)-T\times\sum_{q=q_m}^{q'_m}\mathrm{Re}\tilde{D}_q(0)\right). \tag{5.15}$$

The assumption of *zero* width in the statistical factor, used to get (5.15), is sufficient to obtain the temperature dependence due to η. The wings of statistical factor must be treated very carefully in order to obtain q_m correctly, as we shall see.

According to the proviso under (5.13) we need compute the derivative of (5.15) only with respect to the η dependence. The second term contributes only of order $T^{2/3}$ compared to the first, for $q_m\sim T^{1/3}$, so we neglect it:

$$\frac{d}{dT}\alpha^{(1)}_{\text{boson}}=\frac{2U^2N''(\epsilon_F)}{2\pi N}\left(\sum_q(\gamma q)^2/\Gamma(q)\right)\frac{d\eta}{dT}. \tag{5.16}$$

Now by integrating from $\eta=0$ the first-order differential equation resulting from differentiating (5.10) and using (5.11) and (5.16), one can derive that η has the form

$$\eta=[\tilde{D}_{q\to0}(\omega\equiv0)]^{-1}\equiv\alpha_F+\tfrac{1}{2}\beta_F\tilde{T}\xi. \tag{5.17}$$

The renormalized coefficients are defined by

$$\alpha_F=[\alpha_F^0+\alpha_0^{(1)}+O((T/\epsilon_F)^2\ln(T/\epsilon_F))](1-c)^{-1},$$
$$\beta_F=\beta_F^0(1-c)^{-1}, \tag{5.18}$$

where $c(\leq 0)$ is the sum of the coefficients of $d\eta/dT$ in (5.11) and (5.16) and $\alpha_0^{(1)}$ is the sum of (5.6) and (5.13), all evaluated for $\eta=0$. In $\alpha_0^{(1)}$ one can also neglect the widths ($\sim T$) of statistical factors to lowest order. The $\alpha_0^{(1)}$ and $|c|$ are of order 1.

A. Determination of q_m

We shall determine q_m as described under Eq. (5.13). In order to obtain the proper result for the temperature derivative of the statistical factor in (5.14), we can integrate by parts as before, but the wings of the statistical factor due to the T/ω term must be treated exactly. Specifically, we split the weight of

$$\frac{1}{\pi}\frac{\partial}{\partial\omega}\left[n(\omega)-T/\omega-\tfrac{1}{2}\right]=\frac{T/\pi}{\omega^2+T^2}+\frac{1-\pi}{\pi\omega}g\left(\frac{\omega}{T}\right) \tag{5.19}$$

into a Lorentzian part with the correct asymptotic behavior and a part which gives the correct integrated weight. Here $g(\omega/T)/\omega$ has a width of order T and unit weight but falls off as ω^{-4} at large ω. Integrating (5.14) by parts, we obtain, instead of (5.15),

$$\alpha_{\text{boson}}^{(1)}=\frac{U^2N''(\epsilon_F)}{N}\left(\sum_q^{q'_m}\gamma q\ln[\Gamma(q)+T]+\frac{(1-\pi)}{2\pi}\sum_q^{q'_m}\gamma q\int\frac{dx}{x}\ln[\Gamma^2(q)+x^2T^2]g(x)-T\sum_{q=q_m}^{q'_m}\operatorname{Re}\tilde{D}_q(0)\right). \tag{5.20}$$

If we differentiate the temperature dependence in $\alpha_{\text{boson}}^{(1)}$ not due to η, we obtain a sum of terms proportional to

$$\int_0^{q'_m}\frac{dq\gamma q^3}{\Gamma(q)+T}+\frac{1-\pi}{\pi}\int_0^{q'_m}dq\,\gamma q\int\frac{dx}{x^2}\frac{xg(x)T}{\Gamma^2(q)+x^2T^2}+T\frac{q_m^2}{\eta+\mu_F^2q_m^2}\frac{dq_m}{dT}-\int_{q_m}^{q'_m}\frac{q^2dq}{\eta+\mu_F^2q^2}\,. \tag{5.21}$$

We require that this vanish. The sum of the first and fourth terms produces a contribution of order $q_m-T^{1/3}$ (in suitable units); the second, $-T^{1/3}$; the third, $+T\,dq_m/dT$. Since we can neglect η, it is clear that the solution for q_m which causes (5.21) to vanish is

$$q_m\sim T^{1/3}, \tag{5.22}$$

with a constant of proportionality which can be determined numerically from $g(x)$.

We note that if we had integrated out the sharply peaked (5.19) and used a cutoff approximation $\omega^2\to T^2$ in the argument of the logarithm, we would have missed the first term of (5.21). In this case one would arrive at the erroneous conclusion that one should set $q_m=q'_m=\text{const}$, since the intrinsic $T^{4/3}$ dependence in $\alpha^{(1)}$ from the term analogous to the second term of (5.21) would be negligible compared to $T\xi\sim T$ in (5.1). This difficulty is related to convergence problems which do *not* arise when the η dependence of $\operatorname{Im}\tilde{D}_q(\omega')$ is differentiated. In particular, the steps leading to (5.16) are correct.

The result (5.22) can be understood by the intuitive argument that only modes with damping $\Gamma(q)$ less than the temperature can drive the phase transition. In other words, modes which live longer than the time scale provided by the characteristic thermal excitation energy participate. The modes which damp out more quickly are simply too broad to excite with any degree of certainty. Since $\Gamma(q)\sim q^3$ in the important region of phase space for small η, we immediately obtain $q_m\sim T^{1/3}$.

Now, since ξ goes as q_m, we see that β_F term in (5.1) goes as $T^{4/3}$. For sufficiently low temperatures, this dependence dominates the intrinsic $T^2\ln T$ dependence in $\alpha_{\text{fermion}}^{(1)}$. The driving term for the phase transition is thus entirely isolatable into the β_F term of (5.1). Our picture of the phase transition in weak itinerant ferromagnets as being driven by the classical fluctuations—in a restricted region of phase space—appears to be consistent.

But, as we have seen, the renormalization of the constant values of the α_F and β_F coefficients and the $T^2\ln T$ terms due to the finite-frequency modes is a large effect. The values of $\alpha_0^{(1)}$ and c in Eq. (5.18) are of order 1. Moreover, Eq. (5.18) is still subject to higher-order renormalization effects from finite-frequency modes that are also of order 1. The problem is basically that the sum over the large number of finite-frequency modes (a number of order ϵ_F/T) removes the small parameter (T/ϵ_F) governing the expansion in the classical fluctuations. The conclusion, therefore, is that the GL coefficients cannot be calculated.

However, if as indicated in the preceding discussion, the temperature dependence of α_F and β_F remains weak, we may regard them as parameters to be put into the free-energy functional (2.1). Assuming that some choice of the interaction strength U leads to a weak phase transition, the discussion of Secs. III and IV relying on small parameters carries through.

VI. CONCLUSIONS

We conclude that the Murata-Doniach model for phase transitions in very weak itinerant magnets ($T_C\lesssim 1$ K) should be a useful way to correlate the thermodynamic properties of such a material, should it be found. The transition appears correctly describable as fluctuation driven, in the sense that the mechanism of (1.4) provides the leading temperature dependence in the theory for low T_C in spite of quantum corrections.

To zeroth order, the thermodynamic properties have standard mean field behavior. However, the renormalization of critical ($q \approx 0$) fluctuations and reduction of the thermal population of fluctuations as $T \to 0$ introduces slight ($T^{4/3}$ vs T and $\epsilon^{1/2}$) curvature effects, which may be experimentally observable in regions where perturbation theory in the model is valid. These effects are summarized in the equations listed in Table I and provide the signature for this type of phase transition.

Unfortunately, we also find that one cannot avoid entirely the strong-coupling aspects of the problem, in the sense that certain coefficients, including the Ginsburg-Landau coefficients themselves, cannot be microscopically determined. These (and thus T_C) have to be phenomenologically determined.

APPENDIX

Because of existing discussion on the functional-integral formalism,[21,22] we shall just write down the partition function for the quadratic term in the decomposition of the Hubbard Hamiltonian:

$$H_{\rm int} = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$= \tfrac{1}{2} U \sum_i (n_{i\uparrow} + n_{i\downarrow}) - \tfrac{1}{2} U \sum_i (n_{i\uparrow} - n_{i\downarrow})^2. \quad \text{(A1)}$$

By considering the linear first term incorporated into Z_0, one obtains the partition function Z in terms of the field h representing fluctuations in the z component of the magnetization:

$$\frac{Z}{Z_0} = \int D[h_{qn}] \exp\left[-\sum_{qn} |h_{qn}|^2/2 - \mathcal{F}(h) \right],$$

where

$$D[h_{qn}] = \frac{dh_{00}}{(2\pi)^{1/2}} \prod_{\substack{q>0 \\ n>0}} \left(\frac{d^2 h_{qn}}{(\pi)^{1/2}} \right),$$

and

$$\mathcal{F}(h) = -U\,{\rm Tr}_\sigma \sum_{qn} h_{qn} h_{-q-n} \Phi_\sigma^{(2)}(qn)$$

$$- U^2\,{\rm Tr}_\sigma\, TN^{-1} \sum h_{q_1n_1} h_{q_2n_2} h_{-q_3-n_3} h_{-q_4-n_4} \times \delta_{q_1+q_2,q_3+q_4} \delta_{n_1+n_2,n_3+n_4} \Phi_\sigma^{(4)}$$

$$- U^3\,{\rm Tr}_\sigma T^2 N^{-2} \sum h^6 \Phi_\sigma^{(6)} + \cdots . \quad \text{(A2)}$$

We note the h's are not all independent but satisfy $h_{qn} = h^*_{-q-n}$. The generalized interaction $\Phi_\sigma^{(m)}$ is given from rules of finite-temperature perturbation theory as the closed electron loop for an electron if one spin ($\sigma = \uparrow$ or $\downarrow$) which has m interactions with a scalar external field h_{qn}, which transfers momentum q_i and frequency ω_{n_i} to the electron at the ith vertex.[12] In particular, we include a factor (-1) for the closed fermion loop and a symmetry factor m^{-1}.

As discussed by Schrieffer,[21] the introduction of frequency-dependent fluctuations is necessitated by the noncommutivity of the electron kinetic energy with $H_{\rm int}$. The simplest model of the phase transition arises from ignoring the finite-frequency modes; $\Phi_\sigma^{(m)}$ then becomes particularly simple, but the GL coefficients obtained are only order of magnitude estimates. The nominal values (2.10) are obtained by identifying

$$\tfrac{1}{2}(\alpha_F - 1 + \mu_F^2 q^2 + \cdots) = -U\,{\rm Tr}_\sigma\, \Phi_\sigma^{(2)}(q, 0),$$
$$(1/4!)\,\beta_F = -2U^3\,{\rm Tr}_\sigma \Phi_\sigma^{(4)}(q=0, n=0), \quad \text{(A3)}$$

where

$$\Phi_\sigma^{(2)}(q, n) = (-T/2) \sum_{km} G^\sigma_{n+m,k+q} G^\sigma_{m,k},$$
$$\Phi_\sigma^{(4)}(q=0, n=0) = (-T/4) \sum_{km} (G^\sigma_{km})^4, \quad \text{(A4)}$$

and

$$G^\sigma_{nk} = (\omega_n - \epsilon^\sigma_k)^{-1}.$$

The algebra leading to (2.10) is straightforward.

The effect of a finite external static field $\tilde{H}$ is simply to shift ϵ^σ_k. If G^σ_{nk} is expanded in the field, the effect of $\tilde{H}$ is transferred to a shift in h_{00}, where this appears in $\mathcal{F}(h)$. By change of variables, we obtain the finite-field generalization (2.1).

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