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Low-temperature properties of an almost-localized Fermi liquid

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We calculate the low-temperature corrections to the properties of an almost-localized Fermi liquid in the normal phase caused by the temperature-dependent renormalization of the quasiparticle bandwidth. Our approach provides a natural extension to finite temperatures of the theory of correlated electron systems devised by Brinkman and Rice. Applications to $(V_{1-x}Ti_x)_2O_3$, heavy fermions, and liquid ^{3}He are briefly discussed. The importance of intersite correlations is stressed and discussed in physical terms.

I. INTRODUCTION

It has been pointed out by Anderson and Brinkman,[1,2] and elaborated in detail by Vollhardt,[3] that liquid ^{3}He in the normal phase may be regarded as a system of interacting fermions close to localization (solidification). In particular, an analogy has been drawn[1–3] between ^{3}He behavior and the properties of narrow-band electrons close to the metal-insulator (Mott-Hubbard) transition. The analogy has been pursued formally along the lines proposed by Gutzwiller[4] and developed by Brinkman and Rice.[5] Treatments of both ^{3}He (Refs. 1–3) and of correlated electron systems (Refs. 4 and 5) have been limited to the temperature $T=0$. The extension to $T>0$ has been developed for ^{3}He by Seiler *et al.*,[6] and for correlated electrons by Spałek *et al.*[7,8] However, both groups use a phenomenological expression for the entropy in order to interpolate between the low- and high-temperature limits for ^{3}He and correlated electrons, respectively. The entropy expression reflects a restriction on the number of accessible configurations representing excited states for interacting fermions and leads to localized-moment behavior at ambient temperature.

In this paper we limit ourselves to the low-temperature regime and calculate directly the first nontrivial corrections for $T>0$ to the theoretical results at $T=0$ of Brinkman and Rice,[5] Anderson and Brinkman,[1,2] and Vollhardt.[3] We show that although a treatment in the full temperature range is still lacking, a Fermi-liquid type of analysis at low temperature is feasible. In this way, we avoid the arbitrariness of previous phenomenological approaches,[6–8] though the validity of the present results is limited to the low-temperature regime[9,10] specified herein. As in ordinary Fermi-liquid theory, we assume that near the Fermi energy the electron distribution is adequately described by the Fermi-Dirac function.[11,12]

We use the approach developed recently[10] for the description of discontinuous metal-insulator transitions at $T>0$ in systems of correlated electrons in a half-filled narrow band. The approach is based on a reformulation of the Gutzwiller method[4,5] and relies on a self-consistent calculation of the band narrowing factor for correlated electrons. Here we analyze explicitly the properties of the metallic phase near (but below) the delocalized-localized carrier transition. Thus, this paper is a continuation of our studies[9,10] of itinerant electron systems close to Mott localization within an orbitally nondegenerate narrow-band model. Additionally, we encounter also an almost-localized liquid above the transition (i.e., for $U>U_c$) but only when the band is less than or more than half-filled. The case $n=1$ and $U<U_c$ will be dealt with in Sec. II, while the case $n<1$ and $U\gg U_c$ will be discussed in Sec. III. The results are applied to $(V_{1-x}Ti_x)_2O_3$, liquid ^{3}He, and to heavy-fermion systems. We discuss also the importance of intersite exchange interaction in achieving agreement between theory and experiment.

II. LOW-TEMPERATURE EXPANSION: $U<U_c$

A. Basic assumptions

To set up the basic thermodynamic expressions, we slightly generalize the procedure of Ref. 10. We write the energy of a set of quasiparticles as

$$E_{\mathbf{k}\sigma}=\Phi\varepsilon_{\mathbf{k}}-\sigma\mu_B H\equiv\delta E/\delta\bar{n}_{\mathbf{k}\sigma}\ , \tag{2.1}$$

where E is the total energy of the system of correlated electrons[5,10] with distribution $\bar{n}_{\mathbf{k}\sigma}$, $\varepsilon_{\mathbf{k}}$ is the $\mathbf{k}$-dependent bare particle band energy, $\Phi(\eta)$ is the band-narrowing factor which depends on the average double occupancy $\eta=\langle n_{i\uparrow}n_{i\downarrow}\rangle$ of sites, assumed independent of site index i, $n_{i\sigma}$ is the number operator for occupancy of site i, σ is the spin variable which can assume values $+1(\uparrow)$ or $-1(\downarrow)$; the remaining symbols have their conventional significance. For such a collection of quasiparticles the free energy per site is specified by

$$\frac{F}{N}=\frac{1}{N}\sum_{\mathbf{k}\sigma}E_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}+U\eta+\frac{k_BT}{N}\sum_{\mathbf{k}\sigma}[f_{\mathbf{k}\sigma}\ln f_{\mathbf{k}\sigma}+(1-f_{\mathbf{k}\sigma})\ln(1-f_{\mathbf{k}\sigma})]\ , \tag{2.2}$$

where N is the total number of sites, $f_{\mathbf{k}\sigma}\equiv f(E_{\mathbf{k}\sigma})=\bar{n}_{\mathbf{k}\sigma}$ is the Fermi-Dirac distribution function,[11] U is the magnitude of the intra-atomic Coulomb interaction energy, and the remaining symbols retain their conventional significance. The band narrowing factor is specified by the relation[5]

$$\Phi\equiv\Phi(\eta,m)=\frac{4\eta}{1-m^2}\{1-2\eta+[(1-2\eta)^2-m^2]^{1/2}\}\ , \tag{2.3a}$$

where $m\equiv\langle n_{i\uparrow}-n_{i\downarrow}\rangle$ is the average magnetic polarization per site. In the limit $m\rightarrow 0$ we obtain

$$\Phi=8\eta(1-2\eta)\left[1+m^2\left[1-\frac{1}{4(1-2\eta)^2}\right]\right]\ . \tag{2.3b}$$

In the preceding the quantities Φ and η correspond to the symbols q and d used in Refs. 4–6.

The free energy depends on the particle configuration through η. By a slight generalization of the arguments presented in Ref. 10 (see Appendix C), Eq. (2.2) may be rewritten in the form

$$\frac{F}{N}=\Phi\frac{F_0(T^*,H^*)}{N}+U\eta\ , \tag{2.4}$$

$F_0(T^*,H^*)$ being the free energy of the electron gas at the effective temperature $T^*\equiv T/\Phi$ and in the effective field $H^*\equiv H/\Phi$. A mutual balance between the band ($\Phi F_0<0$) and local-interaction ($U\eta>0$) parts is obtained by imposing the equilibrium condition $\partial F/\partial\eta=0$. Substitution of $\eta=\eta(T)$ obtained from this constraint into (2.2) or (2.4) transforms the free-energy functional into a true free energy. It is this *additional minimization procedure* by which the almost-localized systems are characterized and which leads to a restriction on the motion of individual electrons due to their strong Coulomb interactions. Because of the presence of the term $U\eta$ in Eq. (2.2) or (2.4), the properties of the interacting systems cannot be specified by a simple rescaling of the free-electron gas properties.

Equation (2.4) does not represent the correlated system at arbitrary temperature, since a discontinuous metal-insulator transition at elevated temperature takes place.[10,11] However, as $T\rightarrow 0$, i.e., for $k_BT\ll\Phi|\bar{\varepsilon}|$, where $\bar{\varepsilon}$ is the average bare band energy per site, one can introduce the Sommerfeld expansion to order T^4; a brief description is furnished in Appendices A–C. From the resultant expression one may readily derive the energy E and entropy S of the quasiparticles, and hence, the Helmholtz free energy F. The resulting expression

$$\frac{F}{N}=\Phi\bar{\varepsilon}+U\eta+\frac{\gamma_0}{2\Phi}T^2+\frac{m^2}{4\rho\alpha(T^*)}\Phi-\frac{\pi^4}{36}\frac{(k_BT)^4}{\Phi^3}\left[\frac{7}{5}\rho''-\frac{(\rho')^2}{\rho}\right]+,\ldots\ , \tag{2.5}$$

takes the place of Eq. (2.4). In the preceding, the Sommerfeld free-electron contribution to the heat capacity (per site) is given by $\gamma_0=(2\pi^2k_B^2/3)\rho$, where ρ is the density of states (DOS) per site per spin of noninteracting particles, taken at the Fermi energy ε_F. The magnetic susceptibility of the gas at temperature T^* is given by

$$\chi=\tfrac{1}{2}(g\mu_B)^2\rho\alpha(T^*)\ , \tag{2.6a}$$

with g the Landé factor, μ_B the Bohr magneton,

$$\alpha(T^*)\equiv 1-\frac{\pi 2}{6}\left[\frac{k_BT}{\Phi}\right]^2\left[\left[\frac{\rho'}{\rho}\right]^2-\frac{\rho''}{\rho}\right]+,\ldots\ , \tag{2.6b}$$

and

$$\rho'=(d\rho/d\varepsilon)|_{\varepsilon_F},\ \rho''=(d^2\rho/d\varepsilon^2)|_{\varepsilon_F}\ .$$

The expansion (2.5) along with the conditions for a minimum, namely $\partial F/\partial\eta=0$, and $\partial^2F/\partial\eta^2>0$, constitute the formal structure of our approach. Strictly speaking, Eq. (2.5) represents a free-energy functional. It is transformed into the Helmholtz free energy after substitution of the value $\eta=\eta(T)$ obtained from the minimization procedure. The physical meaning of that procedure, as a way of optimizing the balance between the band and the Coulomb parts of the total energy, has been discussed in Refs. 8–10.

B. Specific heat: $H=0$

Consider first the $m=0$ (i.e., $H=0$) case. On applying the constraint $\partial F/\partial\eta=0$ to Eq. (2.5) we obtain after lengthy algebraic manipulations (outlined in Appendix B) the first nontrivial corrections to η in the form

$$\eta=\eta(T)\equiv\eta_0-aT^2-bT^4\ . \tag{2.7}$$

Introducing (2.7) into (2.3b) we find that

$$\Phi=\Phi_0-8aIT^2-8(bI+2a^2)T^4\ . \tag{2.8}$$

In the preceding expressions the coefficients are given by

$$a\equiv\frac{2\pi^2}{3}\frac{I\rho}{U_c\Phi_0^2}k_B^2\ , \tag{2.9a}$$

and

$$b\equiv\frac{\pi^4I}{U_c\Phi_0^4}k_B^4\left[\frac{16}{9}\frac{\rho^2}{\Phi_0U_c}(1+3I^2)+\frac{1}{6}\left[\frac{7}{5}\rho''-\frac{(\rho')^2}{\rho}\right]\right]\ , \tag{2.9b}$$

with

$$\Phi_0\equiv(1-I^2),\ I\equiv U/U_c,\ \text{and}\ U_c\equiv 8|\bar{\varepsilon}|\ . \tag{2.9c}$$

As $T \rightarrow 0$ the preceding results reduce to those obtained previously.[5,7] Substituting (2.7) and (2.8) into (2.5) we obtain

$$\frac{F}{N} = (1-I)^2\overline{\varepsilon} - \frac{\gamma_0 T^2}{2(1-I^2)} - \frac{1}{4}\frac{\gamma_0^2 T^4}{|\overline{\varepsilon}|\Phi_0^4} I^2 + \frac{\pi^4}{36}\left[\frac{(\rho')^2}{\rho} - \frac{7}{5}\rho''\right]\frac{(k_B T)^4}{\Phi_0^3} . \tag{2.10}$$

The results (2.7) and (2.8) mean that at $T>0$ the band begins to narrow with increasing T, i.e., *precursor localization effects* occur prior to the actual transition with $\Phi \approx 0$. This effect has been obtained before within the phenomenological approach[6-8] and shows up as an increase of effective mass m^*/m_b, where m_b is the effective mass for an electron in a band of width W. According to Eq. (2.8) the enhancement up to T^2 is given by

$$m^*/m_b = \frac{1}{\Phi} \simeq \frac{1}{1-I^2}\left[1 + \frac{2\pi^2 I^2}{3}\frac{(k_B T)^2 \rho}{|\overline{\varepsilon}|(1-I^2)^3}\right] . \tag{2.11}$$

The preceding temperature renormalization of the effective mass disappears if we neglect second- and higher-order effects in U. Note that the enhancement of the effective mass is very large for $I \rightarrow 1$, i.e., close to the metal-insulator transition at $T=0$. Also, the temperature dependence of m^*/m_b due to particle interaction corresponds to a *positive* T^3 contribution to the specific heat; the latter is determined by double differentiation of F with respect to T and has the form

$$C_v = \frac{\gamma_0 T}{\Phi_0} + \frac{3\gamma_0^2 T^3}{|\overline{\varepsilon}|\Phi_0^4} I^2 + \frac{\pi^4}{3}\frac{k_B^4 T^3}{\Phi_0^3}\left[\frac{7}{5}\rho'' - \frac{(\rho')^2}{\rho}\right] , \tag{2.12}$$

where the second positive term appears only when particle interactions are present ($I>0$); the last is the usual higher-order band term for a gas of noninteracting fermions at temperature T^*. For $\Phi_0 \ll 1$ (i.e., for $U \rightarrow U_c - 0$), the term due to the interaction may become dominant, particularly for the systems with a rather featureless density of states near the Fermi energy. Obviously, higher-order terms (not included) will be of opposite sign; thus, the entropy saturates as T increases.

The low-temperature expansion is restricted to the regime $k_B T \ll |\Phi\overline{\varepsilon} + U\eta_0|$; i.e., the total energy, $(1-I)^2\overline{\varepsilon}$ per particle at $T=0$, must be substantially larger than $k_B T$. Near the localization threshold ($U=U_c$) $|\overline{\varepsilon}| \simeq U_c/8$-thus, the temperature regime for which the expansion holds is $k_B T \ll \frac{1}{4}(1-I)U_c$. For example, if $U_c \simeq 4$ eV and $I \approx 0.99$, then the condition $T \ll 10$ K must be satisfied. Therefore, the Fermi-liquid properties specific to the almost-localized systems are in evidence only at low temperatures.

C. Magnetic susceptibility

The temperature renormalization of Φ occurs also in the expression for magnetic susceptibility χ as demonstrated explicitly in Appendix C. Namely, after minimizing the full functional (2.5) with respect to η and taking the limit of small m we obtain the following expression up to order T^2:

$$\eta \equiv \eta(T,m) = \eta_0 - aT^2 - \overline{a}m^2 - bm^2T^2 \tag{2.13}$$

and

$$\Phi \equiv \Phi(T,m) = \Phi_0 - 8I(aT^2 + \overline{a}m^2 + b^2m^2T^2) - 32a\overline{a}m^2T^2 , \tag{2.14}$$

with

$$\overline{a} \equiv \frac{I}{16}\left[\frac{1}{\rho|\overline{\varepsilon}|} + \frac{4(1-I)}{I(1+I)^2} - 8I\frac{1+I/2}{(1+I)^2}\right] . \tag{2.15}$$

The quantity b does not enter the expression for either F or χ because the contributions of various b-dependent terms precisely cancel each other (cf. the discussion in Appendix D). Substituting (2.13) and (2.14) into (2.5) and differentiating twice with respect to the magnetic field we find up to terms of order T^2

$$\chi = \left\{\tfrac{1}{2}(g\mu_B)^2\rho \Big/ \left[\Phi_0\left[1 - \rho U\frac{1+I/2}{(1+I)^2}\right]\right]\right\}\left[1 - d\left\{\pi^2 k_B^2 T^2 \Big/ \left[6\Phi_0^2\left[1 - \rho U\frac{1+I/2}{(1+I)^2}\right]\right]\right\}\right] , \tag{2.16}$$

where

$$d \equiv \left[\frac{\rho'}{\rho}\right]^2 - \frac{\rho''}{\rho} - 32\frac{I^2\rho}{U_c\Phi_0} - 4\frac{I\rho^2}{\Phi_0}\left[4\overline{a} - I - \frac{1}{(1+I)^2}\right] + 8\frac{\rho^2}{\Phi_0}\left[\frac{2I(1-I)(1+I/2)}{1+I} - 8\overline{a}I\right] . \tag{2.17}$$

A particular case of interest arises when $U \rightarrow U_c$, for which we find

$$\chi = \frac{\chi_0(0)}{2(1-I)(1-3\rho U_c/8)}\left[1 - \overline{d}\frac{\pi^2 k_B^2 T^2 \rho}{2U_c(1-I)(1-3\rho U_c/8)}\right] , \tag{2.18}$$

where $\chi_0(0)$ is the susceptibility for noninteracting electrons at $T=0$, and

$$\overline{d} \equiv \frac{U_c}{12\rho(1-I)}\left[\left[\frac{\rho'}{\rho}\right]^2 - \frac{\rho''}{\rho}\right] - \frac{3}{(1-I)^2}\left[1 - \frac{1}{6}\rho U_c\right] . \tag{2.19}$$

In the present model the susceptibility varies with temperature as T^2, and either increases or decreases, depending on whether $\overline{d}$ is positive or negative. χ diverges at $T=0$ either when (i) $\Phi_0 = 1-(U/U_c)^2$ vanishes, i.e., when $U=U_c$, or when (ii)

$$\rho U(1+I/2)/(1+I)^2=1 ,$$

i.e., when the *renormalized Stoner criterion* is met. In case (i) *the Mott transition* to the localized-moment phase takes place[5,10]; in case (ii) the system undergoes a magnetic phase transition. It should be emphasized that the divergence of χ establishes that a true phase transition has taken place in either case.

Inspection of Eq. (2.18) shows that if the DOS at ε_F is large, then transition (ii) precedes (i), whereas if the DOS is small, as when there is a dip in ρ at ε_F, the reverse holds. Furthermore, the localization of electrons is reflected in a change of character of χ from Pauli to Curie behavior[10]; the latter is characterized by a divergent susceptibility in the limit $T=0$. Also, near the transition all terms appearing in the various thermodynamic quantities are renormalized by the factor $\Phi_0^{-n} \sim (1-I)^{-n}$, where $n>1$. The temperature-dependent part diverges as $U \rightarrow U_c$, demonstrating the inapplicability of the low T expansion for $U \geq U_c$. This reflects again the fact that, for $U \geq U_c$, the metallic state is unstable with respect to formation of a state with localized magnetic moments.

The expressions (2.16) and (2.18) may be compared with the results of the paramagnon approach,[17] which specifies the renormalization both of $\chi_0(0)$ and of the term $\sim T^2$ in χ in terms of the Stoner factor $S=(1-U\rho)^{-1}$. The result (2.16) differs from that derived by Béal-Monod[17] in two respects. First, the coefficient d is more complicated since it contains terms which explicitly depend on U. Second, our effective enhancement factor $\tilde{S}$ is equal to

$$\tilde{S}=\left[\Phi_0\left[1-\rho U\frac{1+I/2}{(1+I)^2}\right]\right]^{-1} \equiv \bar{S}\Phi_0^{-1} , \tag{2.20}$$

and approaches the value

$$\tilde{S}=[2(1-I)(1-3\rho U/8)]^{-1} , \tag{2.21}$$

as $U \rightarrow U_c$. We see that both the localization factor Φ_0^{-1}, as well as the renormalized Stoner factor

$$\bar{S}=\left[1-\rho U\frac{1+I/2}{(1+I)^2}\right]^{-1} , \tag{2.22}$$

contribute to the enhancement of magnetic properties. Hence, the value of $\tilde{S}$ will be particularly large for those systems which are *almost magnetic as well as almost localized.* In this sense our approach generalizes the paramagnon theory.

In general, from the critical condition $\bar{S}=\infty$ one can relate the value $U=U_S$ at the Stoner threshold to the value $U=U_c$ at the localization threshold. Namely,

$$U_S=\frac{2U_c}{1-\frac{4}{\rho U_c}}\left[\left[1-\frac{3}{\rho U_c}\right]^{1/2}+\frac{2}{\rho U_c}-1\right] . \tag{2.23}$$

For $\rho U_c \gg 1$ we obtain the Stoner criterion $U_S=1/\rho$. For $U_S < U_c$ the magnetic transition precedes the transition to the localized phase.

III. DISCUSSION OF RESULTS

The principal physical quantities can be represented using the idea of scaling as exemplified by Eq. (2.4). The results are summarized in Table I in implicit form: the

TABLE I. Scaling properties of principal physical quantities of an almost Fermi liquid. The quantities $T^*=T/\Phi$, $H^*=H/\Phi$, and those with subscript zero represent noninteracting particles. Note that the band narrowing factor Φ depends on temperature via $\eta=\eta(T)$ and $m=m(T)$.

Property	Formula for the property	Relation to electron gas properties
Linear specific heat	$C_v=\gamma T$	$\gamma=\gamma_0/\Phi$
Magnetization in low field	$M=\chi_p H$	$\chi_p=\chi_0(T^*)\Big/\left[\Phi\left[1-\rho U\frac{1+I/2}{(1+I)^2}\right]\right]$
Fermi temperature	$T_F=\mu/k_B$	$T_F=T_{F_0}\Phi$
Quasiparticle density of states	$\tilde{\rho}(E)=\frac{1}{N}\sum_k \delta(E-E_k)$	$\tilde{\rho}(E)=\rho(\varepsilon=E/\Phi)/\Phi$
Free energy functional	$F_\eta(T,H)=E-TS$	$F_\eta(T,H)=\Phi F_0(T^*,H^*)+U\eta$
Wilson ratio	$R=\frac{\chi_p}{\gamma}$	$R=\frac{R_0}{1-\rho U\frac{1+I/2}{(1+I)^2}}$

quantity Φ depends still on temperature via the dependence $\eta = \eta(T)$, which is established from the minimization of the free-energy functional $F \equiv F[T;\eta(T)]$ with respect to η.

One may apply this type of theory both to metallic materials close to (but below) the metal-insulator (Mott) transition,[1-3,13] and to heavy-fermion systems. In the former case $U < U_c$ (considered explicitly above), whereas in the latter case we encounter the situation of strongly correlated electrons, $U \gg U_c$, with $\eta \equiv 0$. If a stable metallic state is to exist for $U \gg U_c$ one requires a band filling $n \neq 1$; otherwise one is limited to the Mott insulating state. Thus, two canonical classes of almost-localized metallic systems are found: those for which $U \rightarrow U_c - 0$, and those where $U \gg U_c$ and $n \rightarrow 1$.

Those two types of systems exhibit different properties: for systems where $U \rightarrow U_c - 0$ the renormalized band energy $(\Phi\bar{\varepsilon})$ is comparable to the correlation energy $(U\eta)$, as discussed in detail in Refs. 9 and 10. Two physically distinct temperature regimes may be recognized: (a) $k_B T \ll |\Phi\bar{\varepsilon} + U\eta|$; this is the Fermi-liquid limit discussed earlier; and (b) $k_B T \gtrsim U\eta \sim \Phi|\bar{\varepsilon}|$, i.e., the correlated metal regime. On the other hand, if $U \gg U_c$ (i.e., $U \gg W$) and $n \neq 1$ three distinct regimes exist: (a) $k_B T \ll \Phi|\bar{\varepsilon}|$, the Fermi-liquid limit;[11] (b) $U \gg k_B T \gtrsim \Phi|\bar{\varepsilon}|$, i.e., the limit of a metal with localized moments; (c) $k_B T \gtrsim U$, i.e., the normal metal. The last regime (c) is usually not physically accessible for electrons in solids. Spałek and Wojcik[11] and Rice *et al.*[14] proposed different approaches, both suitable for $U \gg U_c$, which properly describe the transition from the Fermi-liquid to the localized-moment regime.

One additional difference should be noted: for $U \lesssim U_c$ the Hubbard subbands overlap slightly whereas for $U \gg U_c$ they are separated energetically. Hence, the kinetic exchange mechanism between strongly correlated itinerant electrons[15] should be included before any realistic attempt is made to interpret magnetic and other thermodynamic data for heavy fermions, as discussed below. In the remaining part of this section we compare the results for $C_v(T)$ and $\chi(T)$ of Secs. II B and II C, respectively, first with those encountered in $(V_{1-x}Ti_x)_2O_3$ close to the onset of metal-insulator transition,[13,16] and then with the properties of liquid ^{3}He at low temperatures $T \lesssim 0.1$ K. We also briefly relate our results to those obtained by Béal-Monod[17] within spin-fluctuation theory.

A. Case A: The $(V_{1-x}Ti_x)_2O_3$ system

It is well established[13,16] that addition of Ti_2O_3 to V_2O_3 [i.e., in the system $(V_{1-x}Ti_x)_2O_3$ for $x \gtrsim 0.05$] suppresses the metal-insulator transition. The same happens for V_2O_3 at pressures in excess of 25.6 kb or for V_2O_3 containing excess oxygen. Figure 1 shows the striking change in magnetic susceptibility and in specific heat of $(V_{1-x}Ti_x)_2O_3$ at $x \approx 0.05$, which is well reproduced by the present theory for γ and χ. Namely, for $x \approx 0.05$, C/T versus T^2 is linear over a *wider* range than for the remaining compositions, either on the metallic or on the insulating sides of the transition. This effect must be due to the large T^3 term for $x = 0.051$ [cf. Eq. (2.12)]. The presence of a large term $\sim \beta T^3$ cannot be ascribed to phonons since then the results for $x = 0.049$ and $x = 0.051$ should not differ appreciably. Likewise, the temperature dependence of susceptibility changes qualitatively when the metal-insulator transition disappears close to $x \sim 0.05$. The fact that for $x \geq 0.05$ $\chi(T)$ *decreases* with T may mean that the density of states at E_F has a steep dip, as one expects for a system close to the Mott transition. More detailed data of $\chi(T)$ in the low-T regime are needed before a more quantitative analysis is attempted, which also would require inclusion of disorder introduced by substituting V^{3+} cations for Ti^{3+} ions.

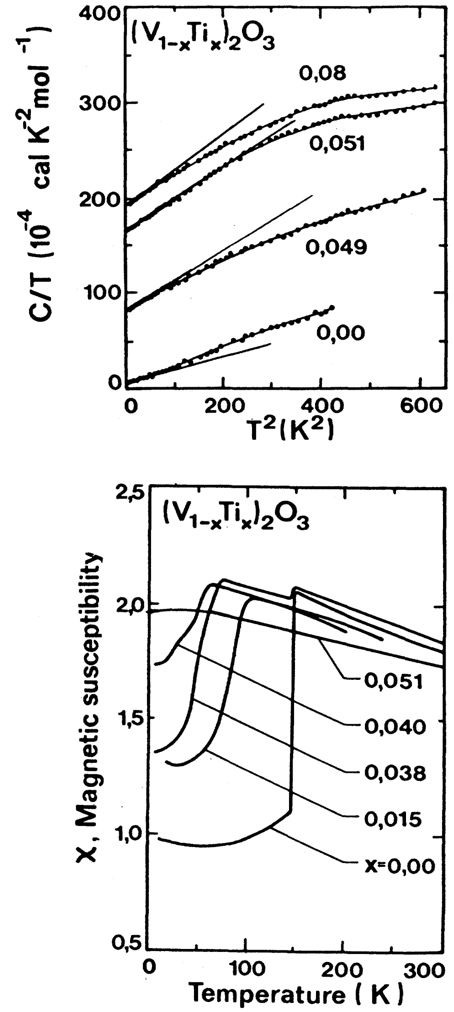

FIG. 1. The temperature dependences of the specific heat (in C/T vs T^2 coordinates) and of the static magnetic susceptibility for the system $(V_{1-x}Ti_x)_2O_3$. Note the pronounced dependence $C/T \sim T^2$ for $x = 0.051$, and the qualitative change of $\chi(T) \sim \chi_0(1 - \bar{a}T^2)$ for this concentration. These properties are characteristic of metallic systems close to the concentration x below which a discontinuous metal insulator transition sets in. The data are taken from Refs. 13 and 16.

The abrupt change in character of the temperature dependence of χ is in accordance with the previous conclusion[8–10] that the electron interaction is a primary factor in driving the *discontinuous* insulator-to-metal transition.

B. Case B: Liquid ^{3}He

We now demonstrate that the application of the present theory to ^{3}He is not as straightforward as for case A. Figure 2 shows plots of C_v/T versus T^2, based on the data by Greywall,[18] for two different molar volumes V. The predicted linear dependence is observed only for $T \lesssim 0.1$ K; similarly, $\chi(T)$ varies as T^2 only in this range.[19] If we write $C_v(T)=\gamma T+\beta T^3$ and $\chi(T)=\chi(0)(1-\bar{d}T^2)$, then a fit to the ^{3}He data requires that $\beta<0$ and $\bar{d}>0$. Note that here β is opposite in sign compared to the case of $(V_{1-x}Ti_x)_2O_3$ (cf. Fig. 1). According to Eqs. (2.12) and (2.18) this can only occur if $(\rho')^2$ is sufficiently large to overcome the correlation-induced type of terms, and/or ρ''/ρ, both of which yield the opposite type inequalities. To meet such requirements the density of states must change drastically at the Fermi level $\varepsilon=\varepsilon_F$. Such a situation might arise for a DOS which has a deep dip at ε_F, just short of the case where a Mott-Hubbard gap opens up.

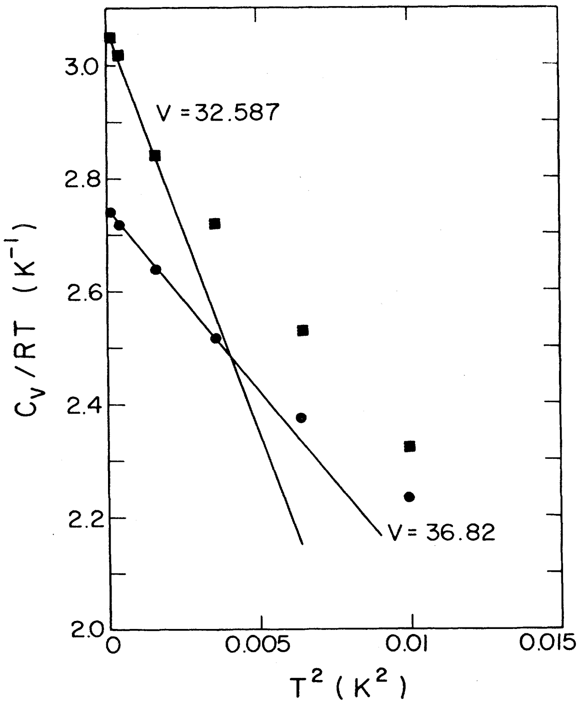

FIG. 2. Plot of C_v/RT vs T^2 for liquid ^{3}He in the normal phase. The data are taken from Ref. 18 (only representative points for $T \le 0.1$ K for two volumes specified are drawn). Note that the term βT^3 is of opposite sign compared to that for $(V_{1-x}Ti_x)_2O_3$ extracted from Fig. 1. This may be regarded as evidence for the presence of a large $T^3\ln(T/\tilde{\Theta})$ term which dominates the positive βT^3 term.

However, an alternative interpretation was advanced by Greywall:[18] by writing

$$C_v=\gamma T+\beta T^3+\delta T^3 \ln T(T/\tilde{\Theta}) ,$$

a fit of the ^{3}He data was achieved over a much wider T range. Similarly, Miyadai *et al.*[20] interpreted their heat-capacity measurements on $NiS_{2-x}Se_x$ in terms of such a model. This raises the question whether the spin-fluctuation theory[17] is more appropriate for these systems or whether the present theory can be expanded to include such an extra term. The latter option may be achieved by inclusion of nonlocal spin fluctuations which will lead to an exchange of paramagnons between almost-localized fermions, as in spin-fluctuation theory.[17]

We gain insight on this problem by starting again with Eq. (2.1) for the energy of quasiparticles. The Hamiltonian for the correlated set is given by

$$\hat{H}_0=\sum_{\mathbf{k}\sigma}(\Phi_\sigma\varepsilon_{\mathbf{k}}-g\mu_B H)n_{\mathbf{k}\sigma}+U_c$$

$$=\sum_{\mathbf{k}\sigma}E_{\mathbf{k}\sigma}n_{\mathbf{k}\sigma}+U\sum_i n_{i\uparrow}n_{i\downarrow} , \tag{3.1}$$

where the intra-atomic interaction was included in the last term. The renormalized quasiparticle energy $E_{k\sigma}$ of the form (2.1) contains only single-site correlation effects, as has been demonstrated in Ref. 7. The first correction to the preceding is provided by an extension of the interactions to nearest neighbors $\langle ij\rangle$, through the terms[21,22]

$$\hat{H}'=\tfrac{1}{2}\sum_{\langle ij\rangle}{}'[J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j+(K_{ij}-\tfrac{1}{4}J_{ij})n_i n_j] , \tag{3.2}$$

where $n_i\equiv\sum_{(\alpha)}n_{i\sigma}$. The preceding forms the direct space analog of the interaction between quasiparticles involving the Pauli spin matrices within the Landau theory.[23,12]

A very interesting case arises when $U\eta$ (>0) in Eq. (2.5) is comparable to, though less than, $\Phi|\bar{\varepsilon}|$. Then the long-range order or collective excitations are determined by the much smaller intersite interactions. Note that by writing $\hat{H}=\hat{H}_0+\hat{H}'$, i.e., by summing (3.1) and (3.2) and treating $\hat{H}'$ to the same degree of approximation as in spin-fluctuation theory (cf. Ref. 17 and references therein), we first attend to the low-energy spin or density fluctuations or to the molecular fields associated with intersite interactions for a frozen configuration of double occupancies (i.e., for a fixed η).[10] The quantity (ηN) is subsequently optimized by minimization of $\langle\hat{H}\rangle$ with respect to η to yield $\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle$ and $\langle n_i n_j\rangle$ in an explicit form. This process ultimately provides expressions similar to those based on spin fluctuation theory,[17] but the procedure is sufficiently involved to require a separate analysis which is beyond the scope of the present paper.

The quantities K_{ij} and J_{ij} contain intersite contributions of higher order in W/U that are neglected in the standard approach.[4,5,9] For example, for $U/W\gg 1$ ($U\gg U_c$) one finds[21]

$$J_{ij}=2t_{ij}^2/(U-K_{ij}) ,$$

if the direct-exchange contribution to J_{ij} is neglected. This expression fails for $U<U_c$, but for a small degree of

overlap of the Hubbard subbands one may estimate the kinetic-exchange integral J_{ij} by replacing U by

$$U_{\text{eff}} = U + W^2/z^2U \ ,$$

where z is the number of nearest neighbors. In other words, the parameter U is renormalized by taking account of virtual hopping processes between the Hubbard subbands. In such a situation,

$$J_{ij} \approx 2t_{ij}^2/(U_{\text{eff}} - K_{ij}) \ ,$$

which is a first-order estimate of J_{ij} associated with multiple virtual hopping processes between the neighboring sites.[15] This expression properly reduces to the limiting cases for the Hubbard model (i.e., for $K_{ij} \equiv 0$). Namely, $J_{ij} \to 2t_{ij}^2/U$ for $U \to \infty$ and $J_{ij} \to U/z$ for $U \to 0$; the latter case reduces correctly to the Hartree-Fock expression for the spin-dependent part of the total energy.

C. Case C: Effect of exchange interactions on the properties of an almost-localized liquid ($U \gg U_c$)

Finally, for comparison we consider the importance of exchange interactions in systems with strongly correlated electrons, i.e., those in the complementary limit $U \gg U_c$. Since for $n = 1$ one has a Mott insulator we restrict ourselves to the case $n < 1$ ($n > 1$ may be handled by the hole formalism). The system is metallic, with $\eta = 0$ and a band narrowing factor[5,7] $\Phi \equiv \Phi_\sigma = (1-n)/(1-n_\sigma)$ and $n_\sigma \equiv \langle n_{i\sigma} \rangle = n/2$ for the case $H = 0$. This band narrowing may be rewritten in the form

$$\Phi_\sigma = (1-n)(1-n_{-\sigma})/(1-n_\sigma)(1-n_{-\sigma}) \ ,$$

or equivalently, as

$$\Phi_\sigma = \frac{1-n}{1-n/2}\left[1 + \frac{\sigma m}{2(1-n/2)} + \frac{m^2}{4(1-n/2)^2}\right] , \qquad (3.3)$$

where, as before, $m \equiv \langle n_{i\uparrow} - n_{i\downarrow} \rangle$. The ground-state energy, inclusive of kinetic exchange interactions between nearest neighbors in the mean-field approximation, is then given by

$$\frac{E_G}{N} = \Phi_0 \bar{\varepsilon}\left[1 + \frac{m^2(2-n/2)}{4(1-n/2)^2}\right] + \frac{m^2\Phi_0}{4\rho} + \frac{Jzm^2}{4} , \qquad (3.4)$$

where

$$\Phi_0 \equiv (1-n)/(1-n/2) \ .$$

The first term specifies the band energy, the second, the work of magnetizing those electrons, whereas the last provides the kinetic-exchange contribution to the total energy.[15] Gathering all terms proportional to m^2 and equating these with $M^2/2\chi(0)$, where M is the magnetization and $\chi(0)$ the zero field susceptibility at $T = 0$, we obtain

$$\chi(0)/\chi_0(0) = \left[\Phi_0\left[1 - \frac{\rho|\bar{\varepsilon}|(2-n/2)}{(1-n/2)^2} + \frac{Jz\rho(1-n/2)}{1-n}\right]\right]^{-1} , \qquad (3.5)$$

where $\chi_0(0)$ is the susceptibility of noninteracting particles in zero field at $T = 0$.

In the absence of a magnetic field the linear specific-heat coefficient is given by $\gamma = \gamma_0/\Phi_0$, where γ_0 is the Sommerfeld coefficient. The dimensionless Wilson ratio is defined by

$$r \equiv \frac{\chi(0)/\chi_0(0)}{\gamma(0)/\gamma_0(0)} = R\frac{\gamma_0(0)}{\chi_0(0)} , \qquad (3.6)$$

for the present case we find

$$r = \left[1 - \frac{\rho|\bar{\varepsilon}|(2-n/2)}{(1-n/2)^2} + \frac{Jz\rho(1-n/2)}{1-n}\right]^{-1} . \qquad (3.7)$$

Here, too, r depends on the strength of the exchange interactions; $r < 1$ only if the last term is larger than the preceding one, which is in agreement with experiment.[24] Equation (3.7) may be compared with the expression for r which can be derived from (2.12) and (2.16) at $T = 0$ for the case $U < U_c$ and with the exchange part $Jzm^2/4$ added to (2.5). Namely,

$$r = \left[1 - U\rho\frac{1 + U/2U_c}{(1+U/U_c)^2} + \frac{Jz}{\Phi_0}\right]^{-1} . \qquad (3.8)$$

The preceding approaches lead to the value $r \to 0$ as $\Phi_0 \to 0$, if $J \neq 0$.

By way of contrast we consider next the limit $T \to \infty$. All strongly correlated systems then exhibit Curie-Weiss type of behavior in the susceptibility. This feature can easily be derived within our approach. It is only necessary to assume that the individual moments in the absence of exchange coupling follow the Curie law, i.e.,

$$\chi_0(T) = n\frac{(g\mu_B)^2\mathcal{T}(\mathcal{T}+1)}{3k_BT} , \qquad (3.9)$$

where $\mathcal{T}$ is the effective spin quantum number. The internal energy of such system of correlated electrons is, within our approach,

$$\frac{E}{N} = \Phi_0\bar{\varepsilon}_\infty + \Phi_0\bar{\varepsilon}_\infty\left[\frac{2-n/2}{4(1-n/2)^2}\right]m^2 + \frac{3m^2k_BT}{8n\mathcal{T}(\mathcal{T}+1)} + \frac{Jz}{4}m^2 , \qquad (3.10)$$

where $\bar{\varepsilon}_\infty$ is the average bare band energy (per site) of the noninteracting electrons at temperature $T^* \to \infty$, given by

$$\bar{\varepsilon}_\infty = 2\int_{-W/2}^{W/2} \varepsilon\rho(\varepsilon)f(\varepsilon) \simeq -\frac{W^2\Phi_0}{24k_BT} . \qquad (3.11)$$

The meaning of the last two terms in Eq. (3.10) is the same as in (3.4). Collecting the terms in m^2 and expressing them again in the form $M^2/2\chi(T)$ we obtain

$$\chi(T) = n\frac{(g\mu_B)^2\mathcal{T}(\mathcal{T}+1)}{3k_B(T+\Theta)} , \qquad (3.12)$$

with

$$\Theta \equiv n\frac{g^2\mathcal{T}(\mathcal{T}+1)}{6k_B}\left[Jz-\Phi_0|\bar{\varepsilon}_\infty|\frac{2-n/2}{(1-n/2)^2}\right] . \tag{3.13}$$

Thus, the susceptibility of correlated electrons contains a temperature-dependent value of Θ since $\bar{\varepsilon}_{in} \sim 1/T$. This introduces a downward trend of the $\chi^{-1}(T)$ curve for decreasing temperature, as is observed for almost all heavy-fermion systems.[24] Only in the asymptotic region of high temperatures does one encounter true Curie-Weiss behavior, with the sign of Θ (>0) corresponding to antiferromagnetic interactions between the particles.

The preceding treatment involves three parameters: W, n, and Jz which can be determined from the experimental values of $\gamma(0)$, and from the asymptotic values of $\chi(T\to 0)$ and $\Theta(T\to\infty)$. As examples we consider the heavy-fermion compounds $CeAl_3$ and $CeCu_6$, for which $\mathcal{T}=\frac{5}{2}$ and $g=\frac{6}{7}$. For $CeAl_3$ the following values are cited[24]: $\gamma(0)=1.62$ J/K^2mol, $\Theta=39$ K and $\chi(0)=36$ memu/mol; if one assumes[25] that at $T=0$ $\mu_{\text{eff}}=\mu_B$ one obtains[26] the following estimates: $n\simeq 0.989$, $m^*/m_b=46.7$, $W^*\equiv\Phi_0 W=33.7$ K, $Jz=36.8$ K, and $r=1.62$. In these expressions m^* is the quasiparticle mass, while m_b is the bare band mass. The bare particle bandwidth is $W=1578$ K. Corresponding values for $CeCu_6$ are $\gamma=1.6$ J/K^2mol, $\Theta=45$ K, $\chi(0)=27$ memu/mol, which yield: $n\simeq 0.977$, $W^*=39.8$ K, $Jz=59.3$ K, $W=770$ K, and $m^*/m_b=22.5$. One should note the very narrow bandwidths and the corresponding very large effective electron masses.[27] For the cited $\gamma(0)$ values, the anticipated m_b/m_0 values would have been 9 and 15, respectively (m_0 is the free-electron mass). Corresponding to the small W^* values, the quantum coherence of the electron states is thermally destroyed for $T\gtrsim 30$ K; this provides an *a posteriori* justification of the assumption that the heavy electrons have atomic moments in the high-temperature regime.[14] Also, the exchange interaction energy $k_B\Theta$ is comparable to quasiparticle bandwidth, suggesting that intersite singlet correlations have an important impact on heavy-fermion properties.

IV. CONCLUDING REMARKS

The principal results of this paper include:

(i) The development for the first time of the low-temperature expansion starting from the Gutzwiller approach, reinterpreted in quasiparticle terms, together with application to the almost-localized system $(V_{1-x}Ti_x)_2O_3$. A one-parameter theory has also been formulated to establish a renormalized Stoner criterion for a phase transition to the ordered magnetic state, and to relate this onset to that of the Mott localization.

(ii) A qualitative discussion of the need to include exchange interactions in real space to achieve closer agreement between the theory of almost-localized Fermi liquid and the experimental results in liquid ^{3}He (Ref. 18) and in some other correlation systems (Ref. 20).

(iii) The estimate of the effective narrow-band parameters $(n, W, m^*/m_0)$ for heavy fermions by including the kinetic-exchange interactions in a theory of strongly correlated, almost-localized systems.

We stress here the difference between the present variational calculation of thermodynamic quantities (via minimization of F with respect to η) and the perturbation treatment of the interaction part within spin-fluctuation theory.[17] The latter is valid close to (but below) the magnetic transition (as determined by the Stoner criterion $U\rho=1$), while our approach is also applicable close to (but below) the metal-insulator transition (as determined by the Brinkman-Rice criterion $U=U_c$).

Further work is needed on the inclusion of the exchange effect in the present theory of almost-localized systems for $U\lesssim U_c$, as well as on the low-temperature expansion inclusive of exchange interactions for $U\gg U_c$.

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APPENDIX A: THE SOMMERFELD LOW-TEMPERATURE EXPANSION

The make the approach self-contained, we provide in this Appendix expressions for several thermodynamic quantities of interest. Any physical quantity expressible in the form

$$Q(T)=2\int_0^W \bar{\rho}(\varepsilon)f(\varepsilon)d(\varepsilon) , \tag{A1}$$

where $\bar{\rho}(\varepsilon)$ is determined by the nature of Q, and

$$f(\varepsilon)\equiv f((\varepsilon-\mu)/k_BT)$$

is the Fermi-Dirac distribution function, may be expanded to powers up to T^4 as[28]

$$Q(T)=2\int_0^\mu \bar{\rho}(\varepsilon)d\varepsilon+\frac{\pi^2}{3}(k_BT)^2\bar{\rho}'(\mu)+\frac{7\pi^4}{180}(k_BT)^4\bar{\rho}'''(\mu) . \tag{A2}$$

The expansion is valid for $k_BT/\mu \ll 1$; the second and third terms involve first and third derivatives of $\bar{\rho}$ evaluated at μ, the Fermi level. This latter quantity also depends on T and must be fixed in the standard manner by specifying the average number of electrons per site

$$n=2\int_0^W \rho(\varepsilon)f(\varepsilon)d(\varepsilon) . \tag{A3}$$

We set $Q=n$ and $\bar{\rho}(\varepsilon)=\rho(\varepsilon)$ in (A2) and for $T\to 0$ set $\mu(T)=\varepsilon_F+\delta\mu(T)$; we further expand $\rho'(\mu)$ in a Taylor series about ε_F (the Fermi level at $T=0$), and finally write the first integral in (A2) with $\bar{\rho}=\rho$ as

$$\int_0^\mu \bar{\rho}(\varepsilon)d\varepsilon=\int_0^{\varepsilon_F+\delta\mu}\rho(\varepsilon)d\varepsilon=\int_0^{\varepsilon_F}\rho(\varepsilon)d\varepsilon+\rho(\varepsilon_F)\delta\mu+\tfrac{1}{2}\rho''(\varepsilon_F)(\delta\mu)^2+\cdots . \tag{A4}$$

Inserting all of the preceding steps into (A2) and collecting terms to order T^4, one obtains a quadratic equation in $\delta\mu$, of which only the root for which $\delta\mu\to 0$ as $T\to 0$ is retained. When the square root is expanded one finds that

$$\delta\mu(T)=-\frac{\pi^2}{6}(k_B T)^2\frac{\rho'}{\rho}+\frac{\pi^4}{72}(k_B T)^4\left[\frac{2\rho'\rho''}{\rho^2}-\frac{7}{5}\frac{\rho'''}{\rho}-\left[\frac{\rho'}{\rho}\right]^3\right] \tag{A5}$$

wherein ρ and its derivatives are evaluated at $\mu=\varepsilon_F$.

Next, set $Q=E(T)/N$ (the internal energy per site), then put $\bar{\rho}\equiv\varepsilon\rho(\varepsilon)$ in (A2), and evaluate the integral by the same technique which led from (A3) to (A5). One then finds

$$\frac{E(T)}{N}=\bar{\varepsilon}+\frac{\pi^3}{3}(k_B T)^2\rho-\frac{\pi^4}{12}(k_B T)^4\left[\frac{(\rho')^2}{\rho}-\frac{7}{5}\rho''\right], \tag{A6}$$

and hence, the heat capacity $C_v=N^{-1}(\partial E/\partial T)_v$, as

$$C_v(T)=\tfrac{2}{3}\pi^2 k_B^2\rho T-\frac{\pi}{3}k_B^4\left[\frac{(\rho')^2}{\rho}-\frac{7}{5}\rho''\right]T^3 . \tag{A7}$$

The entropy is determined via $S(T)/N=\int(C_v/T)dT$ and the free energy is $F/N=E/N-TS/N$. On substituting this result into Eq. (2.4) one obtains Eq. (2.5) with $m=0$. The term in Eq. (2.5) involving m is obtained by the methodology of Appendix C.

APPENDIX B: CALCULATION OF $\eta=\eta(T)$

Apply the condition $\partial F/\partial\eta=0$ to Eq. (2.5). Then for $H=0$ we obtain the expression

$$\left[\varepsilon+\frac{\pi^2}{3\Phi^2}(k_B T)^2\rho+\frac{\pi^4(k_B T)^4}{4\Phi^4}B\right]8(1-4\eta)+U=0 , \tag{B1}$$

where

$$B\equiv\frac{1}{3}\left[\frac{7}{5}\rho''-\frac{(\rho')^2}{\rho}\right] . \tag{B2}$$

Next, expand η in a power series in T:

$$\eta=\eta_0-aT^2-bT^4-cT-dT^3 . \tag{B3}$$

On substituting this power series into (B1) one obtains vanishing values for the coefficients c and d, as well as an equation involving

$$c_0+c_2T^2+c_4T^4=0 ,$$

whose coefficients must also vanish if the above expression is to hold for arbitrary T. The requirement $c_0=c_2=c_4=0$ leads to Eqs. (2.9a) and (2.9b). Insertion of (B3) into Φ yields Eq. (2.8).

APPENDIX C: DERIVATION OF THE FORMULA FOR MAGNETIC SUSCEPTIBILITY

In the presence of a magnetic field the occupation $n_\sigma=\langle n_{i\sigma}\rangle$ in a narrow band half-filled by quasiparticles of energy $E_{\mathbf{k}\sigma}$ is given by

$$n_\sigma=\int_{-W\Phi/2}^{W\Phi/2}dE\tilde{\rho}(E)f_\sigma(E) , \tag{C1}$$

where

$$\tilde{\rho}(E)\equiv\rho(\varepsilon=E/\Phi)/\Phi \tag{C2}$$

and

$$\begin{aligned}f_\sigma(E)&=[1+\exp(E-\tfrac{1}{2}\sigma g\mu_B H-\mu_H)/k_B T]^{-1}\\&=[1+\exp(\varepsilon-\tfrac{1}{2}\sigma g\mu_B H^*-\mu_H^*)/k_B T^*]^{-1}\\&\equiv f\left[\frac{(\varepsilon-\frac{1}{2}\sigma g\mu_B H^*-\mu_H^*)}{k_B T^*}\right]\equiv f_\sigma(x) ,\end{aligned} \tag{C3}$$

with $H^*\equiv H/\Phi$, $T^*\equiv T/\Phi$, $\mu_H^*\equiv\mu_H/\Phi$, $\varepsilon=E/\Phi$. The magnetic polarization $m=\langle n_{i\uparrow}-n_{i\downarrow}\rangle$ per particle is given by

$$m=\int_{-W\Phi/2}^{W\Phi/2}\rho(E)[f_\uparrow(E)-f_\downarrow(E)]dE . \tag{C4}$$

In small applied magnetic fields one may wirte

$$f_\sigma(E)=f\left[\frac{\varepsilon-\mu^*}{k_B T^*}\right]-\frac{1}{2}\frac{\sigma g\mu_B H^*}{k_B T^*}\frac{\partial f}{\partial x}\bigg|_{x=(\varepsilon-\mu^*)/k_B T^*} . \tag{C5}$$

Then

$$m=\frac{g\mu_B H}{\Phi}\int_{-W/2}^{W/2}d\varepsilon\,\rho(\varepsilon)f'\left[\frac{\varepsilon-\mu^*}{k_B T^*}\right]\equiv m_0(T^*,H^*) , \tag{C6}$$

where $f'\equiv\partial f/\partial\varepsilon$. The magnetic susceptibility (per site) is

$$\begin{aligned}\chi(T)=\tfrac{1}{2}g\mu_B m&=\frac{1}{2}\frac{(g\mu_B)^2}{\Phi}\int_{-W/2}^{W/2}d\varepsilon\,\rho(\varepsilon)f'\left[\frac{\varepsilon-\mu^*}{k_B T^*}\right]\\&\equiv\chi_0(T^*)/\Phi .\end{aligned} \tag{C7}$$

The preceding result shows how the Pauli susceptibility of an interacting system at temperature T may be related to that of a quasiparticle system at temperature T^*. The function Φ is itself T dependent, as shown by Eq. (2.14).

Equations (2.6a) and (2.6b) are found by rewriting m as

$$m=(g\mu_B H)\int_0^W d\varepsilon\,\rho(\varepsilon)[f_+(x)-f_-(x)] , \tag{C8}$$

and using the condition for conservation of the number of particles, i.e., the equation

$$n=\int_0^W d\varepsilon\,\rho(\varepsilon)[f_+(x)+f_-(x)] . \tag{C9}$$

The chemical potential is now expanded in terms of H^*,

$$\mu_H(T^*,H^*)=\mu(T^*)+\Delta\mu(T^*,H^*) . \tag{C10}$$

The functions $f_\pm$ in Eq. (C9) are then expanded to yield

$$n=2\int_0^W d\varepsilon\,\rho(\varepsilon)f\left[\frac{\varepsilon-\mu}{k_BT^*}\right]d\varepsilon-2\Delta\mu\int_0^W d\varepsilon\frac{\partial f}{\partial\varepsilon}\bigg|_{\varepsilon-\mu}\rho(\varepsilon)$$
$$+\left[(\Delta\mu)^2+\left[\frac{g\mu_BH^*}{2}\right]^2\right]\int_0^W d\varepsilon\frac{\partial^2 f}{\partial\varepsilon}\bigg|_{\varepsilon-\mu}\rho(\varepsilon)\;. \quad \text{(C11)}$$

The quantity n on the left cancels against the first integral on the right. One can then solve for $\Delta\mu$ to obtain

$$\Delta\mu=(g\mu_BH^*)^2I_2(T^*)/I_1(T^*)\;, \quad \text{(C12)}$$

where

$$I_n(T)\equiv\int_0^W d\varepsilon\frac{\partial^n f}{\partial\varepsilon^n}\bigg|_{\varepsilon-\mu}\rho(\varepsilon)$$
$$=(-1)^n\int_0^W\frac{\partial^n\rho}{d\varepsilon^n}f(\varepsilon)d\varepsilon\;. \quad \text{(C13)}$$

Applying the low-temperature expansion of Appendix A one finds in the limit $H\to 0$

$$\Delta\mu=-(g\mu_BH^*)^2\rho'/8\rho\;. \quad \text{(C14)}$$

Expanding Eq. (C8) in a similar fashion yields

$$m=g\mu_BH[I_1(T^*)-\Delta\mu I_2(T^*)]\;, \quad \text{(C15)}$$

from which one obtains

$$\chi_0(T^*)=\tfrac{1}{2}(g\mu_B)^2I_1(T^*)\;. \quad \text{(C16)}$$

The low-temperature expansion of I_1 then leads to Eq. (2.6b).

Finally, one can use Eq. (C7) to determine the work (per site) involved in magnetizing the quasiparticle system as

$$W=\frac{(g\mu_B)^2m^2}{8\chi(T)}=\frac{m^2(g\mu_B)^2}{8\chi_0(T^*)}\Phi\;. \quad \text{(C17)}$$

On substituting Eq. (C16) into the preceding expression one obtains the magnetic term in (2.5); the Landé factor has been taken as $g=2$.

APPENDIX D: BAND NARROWING FACTOR FOR $H\neq 0$

As for the case $H=0$ we assume that the correlation function $\eta=\eta(T,H)$ can be expanded as

$$\eta=\eta_0-aT^2-\bar{a}m^2-bm^2T^2\;. \quad \text{(D1)}$$

This leads to the following expression:

$$\Phi=\Phi_0-8aIT^2+\left[(1-I)\frac{2I(1+I/2)}{1+I}-8\bar{a}I\right]m^2$$
$$-8\{bI+a[4\bar{a}+I-(1+I)^{-2}]\}m^2T^2\;, \quad \text{(D2)}$$

with

$$\Phi_0=8\eta_0(1-2\eta_0)\;.$$

The free-energy functional up to the order m^2T^2 is then given by

$$\frac{F}{N}=\Phi(m,T)\bar{\varepsilon}+U\eta-\frac{\gamma_0}{2\Phi(m,0)}T^2+\frac{m^2}{4\rho\alpha(T^*)}\Phi(T,0)\;, \quad \text{(D3)}$$

where $\Phi(0,T)$ is given by Eq. (B2), and where $\Phi(m,0)$ is of the form (2.3b), with $\eta=\eta_0$. Substituting (D1) and (D2) into (D3) we obtain

$$\frac{F}{N}=(1-I)^2\bar{\varepsilon}-\frac{\gamma_0T^2}{2(1-I)^2}+\frac{(g\mu_B)^2m^2}{8\chi(T)}\;, \quad \text{(D4)}$$

where $\chi(T)$, the susceptibility per site, is of the form (2.16). Note that the coefficient b does not enter the expression (D4), since it is of higher order.

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