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High-Temperature Magnetic Susceptibility of Interacting Electrons in a Solid. II*

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A new alternative expression for the third virial coefficient for fermions is derived. It is used to deduce an expression for the high-temperature magnetic susceptibility of electrons which interact according to the Hubbard Hamiltonian. The work extends a previous calculation which considered only the second virial coefficient. The results are compared with the Stoner theory of the ferromagnetism of itinerant electrons. The inclusion of the third virial coefficient modifies the usual expression for the susceptibility and indicates an increased tendency toward ferromagnetism.

I. INTRODUCTION

In a previous calculation,[1] the virial-expansion technique was used to examine the magnetic susceptibility of a system of interacting electrons described by the single-band Hubbard Hamiltonian.[2] The virial-expansion technique is applicable to low-density systems and gives an approach to the study of such systems at temperatures higher than the Curie temperature of a possible ferromagnetic transition. The work mentioned above contained a rigorous determination of the second virial coefficient using the methods of solid-state scattering theory.[3] The spin susceptibility which was obtained agreed with the high-temperature susceptibility in the Stoner theory of the ferromagnetism of itinerant electrons.[4] This enabled the establishment of a relation between the paramagnetic Curie temperature of that theory and an element of the t matrix for particle-particle scattering.

The object of this paper is to consider the third virial coefficient for the same system. We are as yet unable to calculate this exactly as was done for the second virial coefficient, and our final result still involves one significant approximation, the nature of which will be specified subsequently.

Several authors have discussed the quantum theory of the third virial coefficient.[5-8] The derivation of this quantity is considered in Sec. II of this paper. The determination of the third virial coefficient b_3 requires information concerning three-particle scattering processes. We employ the Faddeev equations[9] to obtain a concise expression for b_3 [Eq. (2.25)] which contains a free-particle part and a term involving only connected diagrams for three particles. This expression is rigorous, general, and, to the best of our knowledge, original. Fermi statistics are used throughout.

In Sec. III, we consider the theory of the high-temperature spin susceptibility of electrons in a single band interacting according to the Hubbard Hamiltonian. An external magnetic field is added to the Hamiltonian, but only the interaction between the spins and the field is considered. The Hubbard Hamiltonian implies that a pair of electrons interact only when they are in a relative singlet state; and in the case of three particles, interaction occurs only in a doublet state. The external field is included in the virial expansion, and a formal expression for the susceptibility is obtained including three-particle interactions [Eq. (3.14)].

The evaluation of this expression is considered in Sec. IV. At this point, certain approximations are made. The most important of these is that we use a first-order approximation to the solution of the three-particle Faddeev equations, which approximates the t matrix for three particles as the sum of the two-particle t matrices for the different pairs. In the case in which the temperature is large compared to a possible Curie temperature (and to the Fermi energy) but small compared to the bandwidth (the low-density–high-temperature limit), an explicit expression is obtained for the susceptibility in terms of a certain element of the two-body t matrix. The corrections to the formula previously obtained from the second virial coefficient are given, and are seen to favor the occurrence of ferromagnetism in the model.

II. THIRD VIRIAL COEFFICIENT

We will begin by recalling the procedures of the virial expansion.[10] This will establish the notations employed in this paper. The partition function Z of a many-body system may be written in terms of the partition functions of clusters, e.g., $Z_n = \mathrm{Tr}_n [\exp(-\beta H_n)]$ in denoting the number of particles in the cluster and Tr_n denotes the trace over n particle states of the proper symmetry; thus we find

$$Z = 1 + Z_1 e^{\nu} + Z_2 e^{2\nu} + Z_3 e^{3\nu} + \cdots . \tag{2.1}$$

The virial coefficients b_n are defined by the expression

$$\ln Z = Z_1 (e^{\nu} + b_2 e^{2\nu} + b_3 e^{3\nu} + \cdots). \tag{2.2}$$

The b_n's may be expressed in terms of Z_n's by substitution of (2.1) into the left-hand side of (2.2) and equating like powers of e^{ν}:

$$b_2 = (Z_2 - \tfrac{1}{2} Z_1^2)/Z_1, \qquad b_3 = (Z_3 - Z_1 Z_2 + \tfrac{1}{3} Z_1^3)/Z_1, \quad \text{etc.} \tag{2.3}$$

The chemical potential μ is related to ν through the relationship $\nu = \beta\mu$; $\beta = 1/k_B T$, where T is the temperature of the system and k_B is the Boltzmann constant. The quantity e^{ν} is determined by the condition that the number of particles in the system n is fixed:

$$\frac{\partial}{\partial \nu} \ln Z = n = Z_1 (e^{\nu} + 2e^{2\nu} b_2 + 3e^{3\nu} b_3 + \cdots). \tag{2.4}$$

In the low-density limit, e^{ν} can be determined as a power series in n. Actually, the relevant small parameter is essentially the number of particles in a volume equal to the cube of a Debye length. Such a procedure leads us to the well-known equation of state

$$PV \equiv k_B T \ln Z = n k_B T [1 - n b_2/Z_1 - 2n^2 (b_3 - 2b_2^2)/Z_1^2 - \cdots]. \tag{2.5}$$

By computing $\ln Z$ in the presence of an external magnetic field, one may evaluate the magnetic susceptibility of the system also in terms of the virial coefficients. We shall examine this for a special model problem in Sec. III. The possibility of determining these thermodynamic quantities makes the virial series interesting and useful.

We now consider the actual evaluation of the virial coefficients. The second virial coefficient is related to the two-body scattering matrix; in fact, quite generally, the virial coefficients are related to the many-particle scattering matrix as was recently shown by Dashen *et al.*[8] We now follow the method of Callaway and Edwards[1] and relate the third virial coefficient to the connected part of the three-particle scattering matrix, thus obtaining an alternative new expression for b_3. It may be mentioned that the earlier work of Reiner[6] and Baumgartl[7] did not obtain the reduction presented here, nor does the recent elegant work of Dashen *et al.*[8] We confine our attention to fermions, since the application we have in mind is to a system of electrons in a solid. We first rewrite Z_3 and Z_2 in terms of three- and two-particle Green's functions, respectively, and reduce these further in terms of "connected parts" involving scattering matrices and the "interaction free" parts. Let Z_{30} and Z_{20} be the three- and the two-cluster partition functions when there is no interaction. Then we define $(\Delta Z_3) = Z_3 - Z_{30}$ and $(\Delta Z_2) = Z_2 - Z_{20}$. Now, using a well-known trick (see, for example, Ref. 1), we obtain

$$(\Delta Z_2) = \mathrm{Tr}_2 \oint_c \frac{dz}{2\pi i} e^{-\beta z} [G_2(z) - G_{20}(z)], \tag{2.6}$$

where $G_2(z)$ is the two-particle Green's function which satisfies the equation

$$G_2(z) = G_{20}(z) - G_{20}(z) V_2 G_2(z) \equiv G_{20}(z) - G_{20}(z) T_2(z) G_{20}(z). \tag{2.7}$$

$T_2(z)$ is the two-particle t matrix. The contour c in (2.6) encloses all the poles of the integrand:

$$(\Delta Z_2) = -\mathrm{Tr}_2 \oint_c \frac{dz}{2\pi i} e^{-\beta z} G_{20}(z) T_2(z) G_{20}(z)$$

$$= -\sum_{\substack{k_1 k_2 \\ (k_1 > k_2)}} \oint_c \frac{dz}{2\pi i} e^{-\beta z} \frac{\langle k_1 k_2 | T_2(z) | k_1 k_2 \rangle}{[z - E_0(k_1) - E_0(k_2)]^2} \equiv (\Delta Z_2)_c . \quad (2.8)$$

Here k_i's are antisymmetric plane-wave states or Bloch states, as the case may be. Also,

$$Z_{20} = \mathrm{Tr}_2 \oint_c \frac{dz}{2\pi i} e^{-\beta z} G_{20}(z)$$

$$= \sum_{\substack{k_1 k_2 \\ (k_1 > k_2)}} \exp\{-\beta[E_0(k_1) + E_0(k_2)]\} . \quad (2.9)$$

Let us define

$$S_n = \sum_{k_1} e^{-\beta n E_0(k_1)} . \quad (2.10)$$

Then,

$$S_1 \equiv Z_1 = \sum_{k_1} e^{-\beta E_0(k_1)} ,$$

$$S_1^2 = S_2 + 2 \sum_{\substack{k_1 k_2 \\ (k_1 > k_2)}} \exp\{-\beta[E_0(k_1) + E_0(k_2)]\} , \quad (2.11)$$

so that

$$Z_{20} = \tfrac{1}{2}(Z_1^2 - S_2) . \quad (2.12)$$

The expression (2.8) contains all the interactions in it and will be termed "connected" part:

$$Z_2 = (\Delta Z_2)_c + Z_{20} = (\Delta Z_2)_c + \tfrac{1}{2}(Z_1^2 - S_2) \quad (2.13)$$

or equivalently,[1]

$$b_2 = [(\Delta Z_2)_c - \tfrac{1}{2} S_2]/Z_1 . \quad (2.14)$$

A similar procedure leads to the expression

$$(\Delta Z_3) = \mathrm{Tr}_3 \int_c \frac{dz}{2\pi i} e^{-\beta z} [G_3(z) - G_{30}(z)] . \quad (2.15)$$

But now,

$$G_3(z) = G_{30}(z) - G_{30}(z) \left(\textstyle\sum_\alpha V_\alpha\right) G_3(z)$$

$$\equiv G_{30}(z) - G_{30}(z)\, T G_{30}(z) , \quad (2.16)$$

where $\sum_\alpha V_\alpha$ represents the sum of three pairwise interaction potentials, namely, $(V_{12} + V_{23} + V_{31})$, $\alpha = 1$ signifying the pair (23), etc., and T the "formal" T operator associated with $\sum_\alpha V_\alpha$. The Faddeev trick is to rewrite the T operator as a sum $\sum_\alpha T^\alpha$, such that T^α obeys the set of equations[9]

$$T^\alpha = t_\alpha - t_\alpha G_{30}(T^\beta + T^\gamma) , \quad \alpha \neq \beta \neq \gamma . \quad (2.17)$$

Here t_α is the t matrix for the αth pair when the third particle is a spectator. In fact, the Green's function for the αth pair is

$$G_{3\alpha}(z) = G_{30}(z) - G_{30}(z)\, V_\alpha G_{3\alpha}(z)$$

$$\equiv G_{30}(z) - G_{30}(z)\, t_\alpha(z) G_{30}(z) . \quad (2.18)$$

So, the combination

$$G_3(z) - \sum_\alpha G_{3\alpha}(z) + 2 G_{30}(z)$$

$$= [G_3(z) - G_{30}(z)] - \sum_\alpha [G_{3\alpha}(z) - G_{30}(z)]$$

$$= -\sum_\alpha G_{30}(z)(T^\alpha - t_\alpha) G_{30}(z)$$

$$= \sum_{\substack{\alpha\beta \\ (\alpha \neq \beta)}} G_{30}(z) t_\alpha(z) G_{30}(z)\, T^\beta(z)\, G_{30}(z) \equiv G_3^c(z) \quad (2.19)$$

is the connected part of $G_3(z)$, denoted by $G_3^c(z)$. Thus, from (2.15) and (2.19), we obtain

$$(\Delta Z_3) = \mathrm{Tr}_3 \oint_c \frac{dz}{2\pi i} e^{-\beta z} \left(G_3^c(z) + \sum_\alpha G_{3\alpha}(z) - 3 G_{30}(z) \right)$$

$$= (\Delta Z_3)_c + \mathrm{Tr}_3 \sum_\alpha \oint_c \frac{dz}{2\pi i} e^{-\beta z} [G_{3\alpha}(z) - G_{30}(z)] . \quad (2.20)$$

We now use the equation for $G_{3\alpha}$ given by the second line of expression (2.18) above in reducing further the second term in (2.20). We also make use of the fact that in the three-particle frame, the Green's function for the two-particle system given above is independent of the energy of the spectator particle. In other words, $t_\alpha[z + E_\alpha^{(0)}(k_1)]$ is independent of $E_\alpha^{(0)}(k_1)$; so

$$\sum_\alpha \mathrm{Tr}_3 \oint_c \frac{dz}{2\pi i} e^{-\beta z} [G_{3\alpha}(z) - G_{30}(z)]$$

$$= -\frac{1}{3!} \sum_{\substack{k_1 k_2 k_3 \\ (\text{unordered})}} \sum_\alpha \oint_c \frac{dz}{2\pi i} e^{-\beta z} \frac{\langle k_1 k_2 k_3 | t_\alpha(z) | k_1 k_2 k_3 \rangle}{[z - E_\alpha^{(0)}(k_1) - E_\beta^{(0)}(k_2) - E_\alpha^{(0)}(k_3)]^2}$$

$$= -\frac{1}{3!} \sum_{\substack{k_1 k_2 k_3 \\ (\text{unordered})}} \sum_\alpha \oint_c \frac{dy}{2\pi i} \exp\{-\beta[y + E_\alpha^{(0)}(k_1)]\} \frac{\langle k_1 k_2 k_3 | t_\alpha[y + E_\alpha^{(0)}(k_1)] | k_1 k_2 k_3 \rangle}{[y - E_\beta^{(0)}(k_2) - E_\gamma^{(0)}(k_3)]^2} .$$

Noting that $\langle k_1 k_2 k_3 | t_\alpha[y + E_\alpha^{(0)}(k_1)] | k_1 k_2 k_3 \rangle$ is independent of k_1 and $E^{(0)}(k_1)$ and the definition of $(\Delta Z_2)_c$ and Z_1, we obtain

$$\sum_\alpha \mathrm{Tr}_3 \oint_c \frac{dz}{2\pi i} e^{-\beta z} [G_{3\alpha}(z) - G_{30}(z)]$$

$$=\tfrac{1}{3}\sum_{\alpha} Z_1(\Delta Z_2)_c = Z_1(\Delta Z_2)_c \quad . \tag{2.21}$$

Hence,

$$(\Delta Z_3) = (\Delta Z_3)_c + Z_1(\Delta Z_2)_c \quad . \tag{2.22}$$

Putting these together, we obtain

$$b_3 = [(\Delta Z_3)_c + Z_{30} - Z_1 Z_{20} + \tfrac{1}{3} Z_1^3]/Z_1 \quad . \tag{2.23}$$

It may be verified that

$$S_1^3 = S_3 + 3 \sum_{\substack{k_1 k_2 \\ (k_1 > k_2)}} (\exp\{-\beta[E_0(k_1) + 2E_0(k_2)]\} + \exp\{-\beta[2E_0(k_1) + E_0(k_2)]\}) + 6Z_{30} \quad ,$$

where

$$Z_{30} = \sum_{\substack{k_1 k_2 k_3 \\ (k_1 > k_2 > k_3)}} \exp\{-\beta[E_0(k_1) + E_0(k_2) + E_0(k_3)]\} \quad .$$

Also,

$$Z_{20} Z_1 = \tfrac{1}{2}\Big(Z_1^3 - Z_1 \sum_{k_2} \exp[-\beta 2E_0(k_2)]\Big)$$

$$= \tfrac{1}{2}\Big(Z_1^3 - S_3 - \sum_{\substack{k_1 k_2 \\ (k_1 > k_2)}} (\exp\{-\beta[E_0(k_1) + 2E_0(k_2)]\} + \exp\{-\beta[2E_0(k_1) + E_0(k_2)]\})\Big) \, ,$$

so that

$$Z_{30} = \tfrac{1}{6}(Z_1^3 + 2S_3 - 2Z_1 S_2) \quad . \tag{2.24}$$

Consequently,

$$Z_{30} - Z_1 Z_{20} + \tfrac{1}{3} Z_1^3 = \tfrac{1}{3} S_3 \quad . \tag{2.25}$$

Finally, one obtains

$$b_3 = [(\Delta Z_3)_c + \tfrac{1}{3} S_3]/Z_1 \quad . \tag{2.26}$$

This is a new expression for b_3 in terms of $(\Delta Z_3)_c$.

In Sec. IV we shall derive the magnetic susceptibility in terms of the connected parts $(\Delta Z_2)_c$ and $(\Delta Z_3)_c$ for a model Hamiltonian.

III. HIGH-TEMPERATIVE MAGNETIC SUSCEPTIBILITY OF ELECTRONS IN HUBBARD MODEL

We begin by first making a few brief remarks on the Hubbard model. This model in its simplest form proposes the two-particle interaction to be repulsive, independent of wave vector, and *nonzero* only for the singlet spin state of any pair of electrons. Thus, it may be represented by

$$V_{\text{Hubbard}}(12) = -\overline{V}\,\delta^{(3)}(\vec{r}_1 - \vec{r}_2)(\vec{\sigma}_1 \cdot \vec{\sigma}_2 - \tfrac{1}{4}) \quad , \tag{3.1}$$

where $\vec{\sigma}_1$ is the spin vector for particle 1. For a three-particle system the model postulates the mutual interaction to be of the form

$$V(12) + V(23) + V(31) \quad . \tag{3.2}$$

As a consequence of (3.1), the Hubbard model has no interaction among three electrons if their spin state is a quartet. There are two types of doublet states for a three-electron system. The wave functions associated with them will necessarily obey a coupled set of equations.

The magnetic susceptibility of the system is computed by evaluating first the partition function Z in the presence of a small external magnetic field H. The magnetization of the system is then derived by the formula

$$M = \frac{1}{\beta}\frac{\partial}{\partial H} \ln Z(H) \quad . \tag{3.3}$$

The magnetic susceptibility per unit volume is defined by

$$\chi = \lim_{H \to 0} M/VH \quad . \tag{3.4}$$

We will now compute χ for the Hubbard model. Since the two-body interaction alone is in the singlet state and the three-body interaction alone is in the doublet state, enormous simplifications occur in evaluating the various Z_m's in the presence of H:

$$Z_1(H) = (2\cosh\beta\mu_B H)\, Z_1 \quad ,$$
$$S_2(H) = (2\cosh 2\beta\mu_B H)\, S_2 \quad , \tag{3.5}$$
$$S_3(H) = (2\cosh 3\beta\mu_B H)\, S_3 \quad .$$

Here, μ_B is the Bohr magneton. We have

$$(\Delta Z_2)_c(H) = (\Delta Z_2)_c \tag{3.6}$$

independent of H (since it includes only singlets). We also put

$$(\Delta Z_3)_c(H) = (2\cosh\beta\mu_B H)(\Delta Z_3)_c \quad , \tag{3.7}$$

since $(\Delta Z_3)_c$ involves only doublet states. It is plausible that the entire H dependence is contained in the factor $\cosh\beta\mu_B H$, but we have not proved this rigorously. Should this conjecture be false, the addition of terms is easily accommodated in the following analysis. We now have

$$\ln Z(H) = (2\cosh\beta\mu_B H)\, Z_1[e^{\nu} + b_2(H)e^{2\nu} + b_3(H)e^{3\nu} + \dots] \tag{3.8a}$$

with

$$b_2(H) = [(\Delta Z_2)_c - \tfrac{1}{2}(2\cosh 2\beta\mu_B H)S_2]/(2\cosh\beta\mu_B H)Z_1 \quad , \tag{3.8b}$$

$$b_3(H) = [(\Delta Z_3)_c(2\cosh\beta\mu_B H) + \tfrac{1}{3}(2\cosh 3\beta\mu_B H)S_3]/(2\cosh\beta\mu_B H)Z_1 \quad . \tag{3.8c}$$

Hence,

$$\ln Z(H) = (2\cosh\beta\mu_B H) Z_1 e^{\nu} + [(\Delta Z_2)_c - (\cosh 2\beta\mu_B H) S_2] e^{2\nu} + [(\Delta Z_3)_c (2\cosh\beta\mu_B H) + \tfrac{1}{3}(2\cosh 3\beta\mu_B H) S_3] e^{3\nu} + \cdots \quad . \tag{3.9}$$

The number of particles n is determined by the condition[1]

$$n = \left(\frac{\partial \ln Z(H)}{\partial \nu}\right)_H = (2\cosh\beta\mu_B H) Z_1 e^{\nu} + 2[(\Delta Z_2)_c - (\cosh 2\beta\mu_B H) S_2] e^{2\nu} + 3[(\Delta Z_3)_c (2\cosh\beta\mu_B H) + \tfrac{1}{3}(2\cosh 3\beta\mu_B H) S_3] e^{3\nu} + \cdots \quad , \tag{3.10}$$

and the magnetization is given by

$$M = \frac{1}{\beta}\left(\frac{\partial \ln Z(H)}{\partial H}\right) = 2\mu_B \sinh\beta\mu_B H \left[Z_1 e^{\nu} - (2\cosh\beta\mu_B H) S_2 e^{2\nu} + \left((\Delta Z_3)_c + \frac{\sinh 3\beta\mu_B H}{\sinh\beta\mu_B H} S_3\right) e^{3\nu} + \cdots\right] \quad . \tag{3.11}$$

We will not proceed as before to develop the low-density expansion by writing e^{ν} as a power series in n. After some algebra, eliminating e^{ν} in terms of n in the expression for M, we obtain

$$M = n\mu_B \tanh\beta\mu_B H \left[1 - \left(\frac{(\Delta Z_2)_c + S_2}{2Z_1^2 \cosh^2\beta\mu_B H}\right) n + \left(\frac{(\Delta Z_2)_c^2 + 2(\Delta Z_2)_c S_2 - S_2^2}{2Z_1^4 \cosh^4\beta\mu_B H} - \frac{(\Delta Z_2)_c S_2}{Z_1^4 \cosh^2\beta\mu_B H} + \frac{S_3 - (\Delta Z_3)_c}{2Z_1^3 \cosh^2\beta\mu_B H}\right) n^2 + \cdots\right] \quad . \tag{3.12}$$

The magnetic susceptibility is now given by

$$\chi = \frac{n\mu_B^2}{Vk_B T}\left[1 - \left(\frac{(\Delta Z_2)_c + S_2}{2Z_1^2}\right) n + \left(\frac{(\Delta Z_2)_c^2 - S_2^2}{2Z_1^4} - \frac{(\Delta Z_3)_c - S_3}{2Z_1^3}\right) n^2 + \cdots\right] \quad . \tag{3.13}$$

Isolating the connected part from the rest, we may rewrite this in the form

$$\chi = \chi_0 + \frac{\mu_B^2 n}{Vk_B T}\left[-\frac{(\Delta Z_2)_c}{2Z_1^2} n + \left(\frac{(\Delta Z_2)_c^2}{2Z_1^4} - \frac{(\Delta Z_3)_c}{2Z_1^3}\right) n^2 + \cdots\right] \quad . \tag{3.14}$$

We have thus reduced the problem to one of finding $(\Delta Z_3)_c$ since $(\Delta Z_2)_c$ is already computed in I. We will make a few remarks about this aspect of the problem and highlight the essential steps involved in the process.

As stated in the beginning of this section, the Hubbard model allows electrons to interact only in doublet states of the three-electron system. In computing $(\Delta Z_3)_c$ from (2.20), one needs only to consider trace over the doublet states. But as stated earlier, there are two types of doublet states which are degenerate, and this complicates the explicit solution in a straightforward manner. Since one has a nonzero overlap between the two types of doublets, the degeneracy of the states is removed by the model Hamiltonian, thus yielding a coupled set of equations for the doublets. The Faddeev method, therefore, requires certain modification to handle this case. We have set up these equations but have not solved them, however. It seems that they may not be capable of an analytic solution, and perhaps only a numerical analysis may be possible. However, even in the absence of such answers, some conclusions can be reached. These will be indicated in Sec. IV.

IV. EVALUATION FOR A SIMPLE BAND

We will not obtain a more explicit form of the susceptibility subject to certain approximations. We begin by rewriting (3.14) as

$$\chi = (\rho\mu_B^2/k_B T)(1 - F + G) \quad , \tag{4.1}$$

where $\rho = n/V$, and

$$F = \frac{nS_2}{2Z_1^2}\left(1 + \frac{nS_2}{Z_1^2} - \frac{nS_3}{Z_1 S_2}\right) \quad , \tag{4.2}$$

$$G = -\frac{n(\Delta Z_2)_c}{2Z_1^2}\left(1 - \frac{n(\Delta Z_2)_c}{Z_1^2}\right) - \frac{n^2(\Delta Z_3)_c}{2Z_1^3} \quad . \tag{4.3}$$

If G is neglected, the expression for χ reduces to the order considered to be that for noninteracting particles. G contains all the effects of interaction, and we wish to examine it more closely. As mentioned at the end of Sec. III, we are as yet unable to evaluate this completely. The simplest approximation is achieved by retaining only the first-order terms in the Faddeev equations (2.17). In this case $(\Delta Z_3)_c = 0$.

A simple result can then be obtained in the limit of high temperature and low density in which $k_B T$ is large compared to the Fermi energy but small compared to the bandwidth. This is the situation in which the virial expansion is most interesting and is relevant to the case in which a small number of electrons are present in a nearly empty band or in which there are a small number of holes in a nearly full band.

In this case, we may carry over the result of Ref. 1 for $(\Delta Z_2)_c$. From Eq. (83) of that paper, we find that

$$\frac{n(\Delta Z_2)_c}{Z_1^2} = -c\left(\frac{8S_2^2}{Z_1^2}\,\frac{t_0}{\rho k_B T}\right) \quad , \tag{4.4}$$

where c is the ratio of the number of particles to the number of sites, and

$$t_0 = \overline{V}/(1+\tfrac{1}{2}\overline{V}I) \quad . \tag{4.5}$$

$\overline{V}$ is the interaction strength of the Hubbard Hamiltonian,

$$I = \int \frac{g(E)\,dE}{E} \quad , \tag{4.6}$$

where $g(E)$ is the density of states for the band. The quantity t_0 is the two-body t-matrix element for the Hubbard Hamiltonian in the limit $E_F \to 0$.[2,11] We introduce the additional simplifying assumption that $g(E) \sim E^{1/2}$ for energies contributing significantly to S_1 and S_2 (this need not be assumed to hold for the entire band since we assume that the temperature is small compared to the bandwidth). Then $8S_2^2/S_1^2 = 1$ and

$$G = \frac{ct_0}{2k_B T}\left(1 + \frac{ct_0}{k_B T}\right) \tag{4.7}$$

Deviations from the Curie-Weiss law arise as a result of the second term in (4.7) and also from the temperature dependence of the free-particle part F. Suppose for illustrative purposes that F can be neglected. We try to write

$$1/\chi = k_B(T-\Theta)/n\mu_B^2 \quad . \tag{4.8}$$

Then

$$1 - \Theta/T = 1/(1+G) \quad . \tag{4.9}$$

We expand the right-hand side of (4.9), treating $ct_0/k_B T$ as a small parameter, and find

$$k_B\Theta = \tfrac{1}{2}ct_0(1 + ct_0/2k_B T + \cdots) \quad . \tag{4.10}$$

The temperature-independent term is the same as obtained in Ref. 1; the corrections are such as to cause the apparent Curie temperature to increase with decreasing temperature. A graph of $1/\chi$ vs T will tend to curve toward the temperature axis. Qualitatively, an effect of this type is reported in susceptibility data for nickel[12] and nickel-copper alloys.[13] In the analysis of experimental results, it will presumably be necessary, however, to include the temperature dependence of F. The situation may also be too complex for the simple one-band treatment presented here.

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