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Second-Order Green's-Function Theory of the Heisenberg Ferromagnet*

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The coupled Green's-function equations for the Heisenberg ferromagnet are approximated by two coupled differential equations. The approximation agrees at low temperatures with Dyson's spin-wave theory. Computer solutions of spontaneous magnetization for spin $\frac{1}{2}$ and a face-centered cubic lattice represent a better fit to the magnetization of nickel than that afforded by an earlier first-order theory. Compared with the latter, the parameter $\theta_c = kT_c/J$ for cubic lattices and for spin $\frac{1}{2}$ is found to give closer agreement with values obtained from high-temperature series expansions. The renormalized exchange interaction, calculated for all temperatures below the Curie temperature, falls off with increasing temperature, and apparently represents a poorer fit to the experimental data than the results of the first-order theory.

I. INTRODUCTION

In this paper we apply the double-time temperature-dependent Green's-function technique to the Heisenberg Hamiltonian, utilizing a second-order approximation, in which the set of coupled Green's-function equations is approximated by two coupled differential equations. This represents an improvement over a previous investigation[1] which approximated the coupled set of Green's function equations with a single first-order differential equation, in a manner introduced by Callen.[2] Our approximation agrees at low temperatures with Dyson's spin-wave theory.[3] Computer solutions indicate that the transition to spontaneous magnetization found in the earlier first-order approximation in Ref. 1 persists in the present improved approximation. The theoretical zero-field magnetization-versus-temperature curve for $S=\frac{1}{2}$ represents an improved fit to the experimental magnetization of nickel compared to the result obtained from first-order theory. The Curie point $\theta_c = kT_c/J$ for the face-centered cubic lattice is found to be equal to 4.00, in exact agreement with the theoretical value of θ_c given by Rushbrooke *et al.*[4] from a high-temperature series. The renormalized exchange interaction J_{eff} is calculated for all temperatures below T_c. At $T=T_c$, J_{eff} is not zero as first-order theory predicts, but is still about 55% of its zero-temperature value. In Sec. II we derive the first two coupled Green's-function equations whose solution constitutes the present approximation. The details of the solution are given in Appendix I, and utilized in Sec. III to obtain expressions for the renormalized magnon energies and lifetimes. Section IV contains the derivation of the spin-spin correlation functions, the spontaneous magnetization, and the magnetic specific heat at low temperatures. Here we demonstrate the equivalence with Dyson's theory. Section V is devoted to obtaining numerical results at general temperatures for the spontaneous magnetization and the effective exchange interaction.

II. TEMPERATURE-DEPENDENT GREEN'S FUNCTIONS

The Heisenberg Hamiltonain is given by

$$\mathcal{H} = -\mu H \sum_j S_j^z - \sum_i \sum_j J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j , \tag{1}$$

where the sums over i and j range over all of the atoms in the solid. The first term on the right-hand side of this equation represents the interaction of an externally applied magnetic field H, with the magnetic moment μ associated with each unit of spin ($\hbar/2$). The direction of H defines the z direction in space and S_j^z is the z component of the total spin angular momentum operator for atom j. The last term of Eq. (1) represents the spin-spin coupling of each spin to other spins in the solid.

It is assumed that the wave-function overlap is appreciable only for nearest-neighbor atoms so that Eq. (1) can be approximated by replacing J_{ij} by a nonzero constant exchange energy J if i and j are nearest neighbors and by zero otherwise. This is believed to be a good first approximation to Eq. (1) for nonconducting ferromagnets.

If $J>0$ the above Hamiltonian describes a ferromagnet. The system has a well-ordered ground state with all spins aligned in the z direction, since this configuration gives the lowest possible energy for the system.

Let $A(t)$ and $B(t)$ be any pair of operators in the Heisenberg representation which can be defined for this system. The advanced and retarded Green's

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[1] J. Copeland and H. A. Gersch, Phys. Rev. **143**, 236 (1966); J. Copeland, Ph.D. thesis, Georgia Institute of Technology, 1965 (unpublished).

[2] H. B. Callen, Phys. Rev. **130**, 890 (1963).

[3] F. J. Dyson, Phys. Rev. **102**, 1217 (1956); **102**, 1230 (1956).

[4] G. A. Baker, H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Phys. Letters **20**, 146 (1965).

functions based on these operators are

$$\begin{aligned} G_r(t,t') &= -i\theta(t-t')\langle[A(t),B(t')]\rangle\,, \\ G_a(t,t') &= -i\theta(t'-t)\langle[A(t),B(t')]\rangle\,, \\ \theta(t-t') &= 0 \quad \text{if} \quad t'>t\,, \\ &= 1 \quad \text{if} \quad t>t'\,. \end{aligned} \tag{2}$$

The square brackets represent the commutator or anticommutator:

$$[A,B]=AB-\eta BA\,, \tag{3}$$

where $\eta=1$ for commutator and $\eta=-1$ for anticommutator. The angular brackets in Eq. (2) indicate an average over a canonical ensemble. That is

$$\begin{aligned} \langle A(t)\rangle &= Z^{-1}\,\mathrm{Tr}[e^{-\beta\mathcal{H}}A(t)]\,, \\ Z &= \mathrm{Tr}(e^{-\beta\mathcal{H}})\,. \end{aligned} \tag{4}$$

The symbol β denotes the reciprocal of the product of Boltzmann's constant and the absolute temperature, Z is the partition function, and Tr indicates the trace of a matrix.

In calculating physical properties of the system it is necessary that the average over the canonical ensemble of products of operators A and B be known. These averages are known collectively as time correlation functions. The two simplest correlation functions are

$$\begin{aligned} F_{AB}(t) &= \langle A(t)B(0)\rangle\,, \\ F_{BA}(t) &= \langle B(0)A(t)\rangle\,. \end{aligned} \tag{5}$$

These time correlation functions can be obtained if the Green's functions (2) are known. The direct connection can be established by means of a spectral representation of the functions involved.[5] The result is

$$\begin{aligned} F_{AB}(t)=\langle A(t)B(0)\rangle = \frac{i\eta}{2\pi}\lim_{\epsilon\to 0+}\int_{-\infty}^{\infty}\frac{e^{-i\omega t}}{\eta-e^{-\beta\omega}} \\ \times[G(\omega+i\epsilon)-G(\omega-i\epsilon)]d\omega\,. \end{aligned} \tag{6}$$

The Green's functions are determined from their equations of motion. These equations are formed by

$$\begin{aligned} i(d/dt)G_r(t) = \delta(t)\langle[A(t),B(0)]\rangle \\ +\theta(t)\langle[(d/dt)A(t),B(0)]\rangle\,. \end{aligned} \tag{7}$$

The equations of motion for the Heisenberg operators are known to be

$$i(d/dt)A(t)=[A(t),\mathcal{H}]\,. \tag{8}$$

The poles of the spectral function $G_r(E)$,

$$G_r(E)=\frac{1}{2\pi}\int_{-\infty}^{\infty}G_r(t,0)e^{iEt}dt\,,$$

are connected to the energy states of the system,

$$\begin{aligned} G_r(E) = \lim_{\epsilon\to 0+} Z^{-1}\sum_n\sum_m \\ \times\frac{\langle C_m|B(0)|C_n\rangle\langle C_n|A(0)|C_m\rangle(e^{-\beta E_n}-\eta e^{-\beta E_m})}{E-(E_m-E_n)+i\epsilon}\,. \end{aligned} \tag{9}$$

Thus the "poles" for $G_r(E)$ occur at $E=E_m-E_n$, which corresponds to the energy difference between states m and n.

The thermodynamic behavior of this system will be determined by the use of the temperature-dependent double-time Green's function defined by Eq. (2). The choice of the operators A and B is made to effect a quasiparticle description for the system. The retarded Green's function, defined for the Hamiltonian (1), is given by

$$G_1(j,t)=-i\theta(t)\langle[S_j^-(t),S_0^+(0)]\rangle\,, \tag{10}$$

where the spin raising and lowering operators S_j^-, S_j^+ are defined by

$$S_j^\pm=S_j^x\pm iS_j^y\,, \tag{11}$$

where S_j^x and S_j^y are the x and y components, respectively, of S_j. The operators $S_j^\pm$, S_j^z satisfy the equal-time commutation rules

$$[S_j^+,S_i^-]=2S_j^z\delta_{ij}\,, \tag{12}$$

$$[S_j^\pm,S_i^z]=\mp S_j^\pm\delta_{ij}\,. \tag{13}$$

The choice of the commutator ($\eta=1$) here is based on the commutator of (12). The spin-deviation operators are not pure boson operators, since the commutator is not a c number. However, at low temperature this commutator approximates a boson character since the operator S_j^z will be about equal to the spin S for the low-lying states. Thus it might be expected that this system could be described in terms of boson quasiparticles with corrections made for the non-c-number commutator.

The equation of motion for $G_1(j,t)$, obtained from the derivatives of the spin raising and lowering operators

$$\begin{aligned} i(\partial/\partial t)S_j^-(t) = -\mu H S_j^-(t) \\ +2J\sum_p[S_j^z(t)S_{j+p}^-(t)-S_j^-(t)S_{j+p}^z(t)]\,, \end{aligned} \tag{14}$$

$$\begin{aligned} i(\partial/\partial t)S_j^+(t) = \mu H S_j^+(t) \\ +2J\sum_p[S_j^+(t)S_{j+p}^z(t)-S_j^z(t)S_{j+p}^+(t)] \end{aligned} \tag{15}$$

is given by

$$\begin{aligned} [i(\partial/\partial t)+\mu H]G_1(j,t) = -2\langle S^z\rangle\delta(t)\delta_{j,0} \\ +2Ji\theta(t)\sum_p\langle[S_j^-(t)S_{j+p}^z(t) \\ -S_j^z(t)S_{j+p}^-(t)\,,\ S_0^+(0)]\rangle\,. \end{aligned} \tag{16}$$

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[5] D. N. Zubarev, Usp. Fiz. Nauk 71, 71 (1960) [English transl.: Soviet Phys.—Uspekhi 3, 320 (1960)].

As a result of the commutation rules (12), (13) the terms in the sum are not all G_1 functions. These terms couple the G_1 function to a higher order Green's function G_2. This coupling is based on the identity between S_j^z and the operator $S_j^- S_j^+$, which can be verified from Eqs. (11), (12), and (13).

$$S_j^-(t)S_j^+(t)=(S-S_j^z)(S+S_j^z+1). \tag{17}$$

For $S=\frac{1}{2}$, Eq. (17) reduces to

$$S_j^z=S-S_j^-S_j^+. \tag{18}$$

From here on the equations are restricted to the case $S=\frac{1}{2}$ because of the explicit use of (18). The G_1 equation becomes

$$[i(\partial/\partial t)+\mu H]G_1(j,t)+2JS\sum_\rho [G_1(j,t)-G_1(j+\rho,t)]$$
$$=-2\langle S^z\rangle\delta(t)\delta_{j,0}+2J\sum_\rho$$
$$\times[G_2(j,j+\rho,j+\rho,t)-G_2(j+\rho,j,j,t)], \tag{19}$$

where G_2 is defined by

$$G_2(1,2,3,t)=-i\theta(t)\langle[S_1^-(t)S_2^-(t)S_3^+(t),S_0^+(0)]\rangle. \tag{20}$$

The numerals 1, 2, 3 will henceforth represent the lattice vectors j_1, j_2, j_3.

The equation of motion G_2 is then

$$i(\partial/\partial t)G_2(1,2,3,t)=\delta(t)\langle[S_1^-S_2^-S_3^+,S_0^+]\rangle-i\theta(t)\langle[A(t),S_0^+(0)]\rangle, \tag{21}$$

where

$$A(t)=[S_j^-(t),\mathcal{H}]S_2^-(t)S_3^+(t)+S_1^-(t)[S_2^-(t),\mathcal{H}]S_3^+(t)+S_1^-(t)S_2^-(t)[S_3^+(t),\mathcal{H}]. \tag{22}$$

Then using Eqs. (14) and (15) the equation of motion for the G_2 function is

$$[i(\partial/\partial t)+\mu H]G_2(1,2,3,t)=-2\delta(t)[\delta_{1,0}S\langle S_2^-S_3^+\rangle+\delta_{2,0}S\langle S_1^-S_3^+\rangle-\delta_{1,0}\delta_{2,0}\langle S_1^-S_3^+\rangle-\delta_{1,0}\langle S_2^-S_0^-S_0^+S_3^+\rangle$$
$$-\delta_{2,0}\langle S_1^-S_0^-S_0^+S_3^+\rangle]+2Ji\theta(t)\sum_\rho\langle[(S_1^-(t)S_{1+p}^z(t)-S_1^z(t)S_{1+p}^-(t))S_2^-(t)S_3^+(t),S_0^+(0)]\rangle$$
$$+2Ji\theta(t)\sum_\rho\langle[S_1^-(t)(S_2^-(t)S_{2+\rho}^z(t)-S_2^z(t)S_{2+\rho}^-(t))S_3^+(t),S_0^+(0)]\rangle$$
$$-2Ji\theta(t)\sum_\rho\langle[S_1^-(t)S_2^-(t)(S_{3+p}^z(t)S_3^+(t)-S_{3+p}^+(t)S_3^z(t)),S_0^+(0)]\rangle. \tag{23}$$

Again because of the commutation (12), (13) G_2 is coupled to a higher order Green's function. Using Eq. (18), the above equation becomes

$$[i(\partial/\partial t)+\mu H]G_2(1,2,3,t)+2JS\sum_\rho[G_2(1,2,3,t)\{1-2\delta_{2,1+\rho}\}-G_2(1+\rho,2,3,t)\{1-2\delta_{1,2}\}-G_2(1,2+\rho,3,t)$$
$$+G_2(1,2,3+\rho,t)]=-2\delta|t)\{\delta_{1,0}S\langle S_2^-S_3^+\rangle+\delta_{2,0}S\langle S_1^-S_3^+\rangle-\delta_{1,0}\delta_{2,0}\langle S_1^-S_3^+\rangle-\delta_{1,0}\langle S_2^-S_0^-S_0^+S_3^+\rangle$$
$$-\delta_{2,0}\langle S_1^-S_0^-S_0^+S_3^+\rangle\}+2J\sum_\rho[G_3(1,2,1+\rho,1+\rho,3,t)-G_3(1+\rho,2,1,1,3,t)+G_3(1,2,2+\rho,2+\rho,3,t)$$
$$-G_3(1,2+\rho,2,2,3,t)+G_3(1,2,3,3,3+\rho,t)-G_3(1,2,3+\rho,3+\rho,3,t)], \tag{24}$$

where

$$G_3(1,2,3,4,5,t)=-i\theta(t)\langle[S_1^-(t)S_2^-(t)S_3^-(t)S_4^+(t)S_5^+(t),S_0^+(0)]\rangle. \tag{25}$$

The equation of motion for G_3 can be derived by the same method used above to obtain the equations of motion for G_1 and G_2.[6]

It is clear that by continuing this process an infinite set of coupled differential equations will be generated. In order to determine G_i the Green's function G_{i+1} must be known. This set of differential equations is restricted to the case $S=\frac{1}{2}$ since Eq. (18) was used to produce the coupling.

III. SECOND-ORDER CALCULATION

Setting $G_i=0$ for $i>1$ in Eq. (19) yields spin-wave-theory results. Expanding G_2 in terms of G_1 represents the first-order theory previously treated.[1,2]

The second-order calculation begins with solving for G_2 as given by Eq. (24) with $G_3=0$. That is,

$$[i(\partial/\partial t)+\mu H]G_2(1,2,3,t)+2JS\sum_\rho\{G_2(1,2,3,t)[1-2\delta_{2,1+\rho}]-G_2(1+\rho,2,3,t)[1-2\delta_{1,2}]-G_2(1,2+\rho,3,t)$$
$$+G_2(1,2,3+\rho,t)\}=-2\delta|t)[\delta_{1,0}S\langle S_2^-S_3^+\rangle+\delta_{2,0}S\langle S_1^-S_3^+\rangle-\delta_{1,0}\delta_{2,0}\langle S_1^-S_3^+\rangle]. \tag{26}$$

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[6] J. F. Cooke, Ph.D. thesis, Georgia Institute of Technology, 1965 (unpublished).

The quadruple-product terms in the inhomogeneous term on the right-hand side of (26) can be dropped for the case $S=\frac{1}{2}$. This can be done without destroying the property that if $1=2$ the total equation reduces to zero as it should, since $S_j^{\pm}S_j^{\pm}=0$ for the spin-$\frac{1}{2}$ system.

This equation is Fourier inverted to obtain a solution. $G_2(1,2,3,t)$ may be represented by

$$G_2(1,2,3,t)=\frac{1}{2\pi N^3}\sum_{\mathbf{p}1}\sum_{\mathbf{p}2}\sum_{\mathbf{p}3}\int_{-\infty}^{\infty} G_2(p_1,p_2,p_3,\omega)e^{-i\omega t}e^{i[\mathbf{p}_1\cdot\mathbf{j}_1+\mathbf{p}_2\cdot\mathbf{j}_2+\mathbf{p}_3\cdot\mathbf{j}_3]}d\omega\,. \tag{27}$$

Then Eq. (19) becomes

$$[\omega+\mu H+2JS(\gamma_0-\gamma_p)]G_1(p,\omega)=-2\langle S^z\rangle+\frac{2J}{N^2}\sum_{p1}\sum_{p2} G_2(p_1,p_2,p-p_1-p_2,\omega)[\gamma_{p-p1}-\gamma_{p2}] \tag{28}$$

and (26) becomes

$$\begin{aligned}[\omega+\mu H+J(\gamma_0-\gamma_{p1}-\gamma_{p2}+\gamma_{p3})]G_2(p_1,p_2,p_3,\omega)=&-S_{p3}[N(\delta_{p1,-p3}+\delta_{p2,-p3})-2]\\&+(2J/N)\sum_{p'} G_2(p',p_1+p_2-p',p_3,\omega)(\gamma_{p1-p'}-\gamma_{p'})\,,\end{aligned} \tag{29}$$

where

$$\begin{aligned}S_p&=\sum_n \langle S_0^-S_n^+\rangle e^{-i\mathbf{p}\cdot\mathbf{n}}\,,\\ \gamma_p&=\sum_\rho e^{i\mathbf{p}\cdot\rho}\,.\end{aligned} \tag{30}$$

The solution of Eq. (29) for G_2, obtained in Appendix I is given by Eq. (I14), and contains as a factor the term $G_1^0(p\cdot\omega)=-2\langle S^z\rangle/(\omega+E_p^0)$. A renormalization of the magnon energies will now be effected by replacing $G_1^0(p,\omega)$ by $G_1(p,\omega)$, which amounts to replacing the noninteracting magnon energy E_p^0 which appears in the denominator of $G_1^0(p,\omega)$ by the renormalized energy E_p. Arguments in support of this procedure are given at the end of this section.

With the replacement $G_1^0\to G_1$, the inversion of the solution given by Eq. (I14) to space-time coordinates gives

$$G_2(1,2,3,t)=\langle S_1^-S_3^+\rangle G_1(2,t)+\langle S_2^-S_3^+\rangle G_2(1,t)+U(1,2,3,t)\,. \tag{31}$$

If the last term in this equation is neglected, (31) reduces to the well-known Hartree-Fock approximation of the G_2 function. The function U is thus a correction term to the Hartree-Fock terms which contains the dynamical interactions of the magnons.

Substitution of $G_2(p_1,p_2,p-p_1-p_2,\omega)$, given in Appendix I by Eqs. (I14) and (I15), into (28) gives the renormalized equation

$$[\omega+E_p^0-E_p^{\mathrm{HF}}-W(p,\omega)]G_1(p,\omega)=-2\langle S^z\rangle+V(p,\omega)\,, \tag{32}$$

where

$$\begin{aligned}V(p,\omega)=&\frac{4v^2J}{(2\pi)^6}\int\int\frac{S_{p-p1-p2}(\gamma_{p-p1}-\gamma_{p1})}{\omega+E_{p1}{}^0+E_{p2}{}^0-E_{p-p1-p2}{}^0}d^3p_1d^3p_2\\&+\frac{4v^3J^2}{(2\pi)^9}\int\int\int\frac{S_{p-p1-p2}(\gamma_{p-p1}+\gamma_{p-p2}-\gamma_{p1}-\gamma_{p2})(\gamma_{p1-p'}-\gamma_{p'})d^3p_1d^3p_2d^3p'}{(\omega+E_{p1}{}^0+E_{p2}{}^0-E_{p-p1-p2}{}^0)(\omega+E_{p'}{}^0+E_{p1+p2-p'}{}^0-E_{p-p1-p2}{}^0)}\\&+\frac{2J^2v^3}{(2\pi)^9}\int\int\int\frac{D_{\rho'}{}^{\rho}\alpha_\rho(p')h_{\rho'}(p_1+p_2,p-p_1-p_2,\omega)(\gamma_{p-p1}+\gamma_{p-p2}-\gamma_{p1}-\gamma_{p2})(\gamma_{p1-p1'}-\gamma_{p'})d^3{}_{p1}d^3p_2d^3p'}{(\omega+E_{p1}{}^0+E_{p2}{}^0-E_{p-p1-p2}{}^0)(\omega+E_{p'}{}^0+E_{p1+p2-p'}{}^0-E_{p-p1-p2}{}^0)}\,,\end{aligned} \tag{33}$$

and

$$\begin{aligned}E_p{}^{\mathrm{HF}}&=\frac{2Jv}{(2\pi)^3}\int\frac{S_{p'}}{2\langle S^z\rangle}(\gamma_0-\gamma_p-\gamma_{p'}+\gamma_{p-p'})d^3p'\,,\\ E_p{}^0&=J(\gamma_0-\gamma_p)\,,\end{aligned} \tag{34}$$

$$\begin{aligned}W(p,\omega)=&\frac{2v^2J^2}{(2\pi)^6}\int\int\frac{S_{p-p1-p2}(\gamma_{p1-p}+\gamma_{p2-p}-\gamma_p-\gamma_{p-p1-p2})(\gamma_{p-p1}+\gamma_{p-p2}-\gamma_{p1}-\gamma_{p2})}{2\langle S^z\rangle(\omega+E_{p1}{}^0+E_{p2}{}^0-E_{p-p1-p2}{}^0)}d^3p_1d^3p_2\\&+\frac{2v^3J^2}{(2\pi)^9}\sum_\rho\sum_{\rho'}\int\int\int\frac{D_{\rho'}{}^{\rho}\alpha_\rho(p')g_{\rho'}(p-p_1-p_2,p)(\gamma_{p-p1}+\gamma_{p-p2}-\gamma_{p1}-\gamma_{p2})(\gamma_{p1-p'}-\gamma_{p'})d^3p_1d^3p_2d^3p'}{2\langle S^z\rangle D(\omega+E_{p1}{}^0+E_{p2}{}^0-E_{p-p1-p2}{}^0)(\omega+E_{p'}{}^0+E_{p'-p1-p2}{}^0-E_{p-p1-p2}{}^0)}\,.\end{aligned} \tag{35}$$

The analytic continuation of $G_1(p,\omega)$ into the complex ω plane is then given by

$$[\omega+\epsilon(p,\omega)\pm i\tau^{-1}(p,\omega)/2]G_1(p,\omega\pm i\epsilon)=-2\langle S^z\rangle+V(p,\omega\pm i\epsilon)\,, \quad (36)$$

where

$$\epsilon(p,\omega)=E_p{}^0-E_p{}^{\mathrm{HF}}-\mathrm{Re}[W(p,\omega)]\,, \quad (37)$$

$$\tau^{-1}(p,\omega)/2=\mathrm{Im}[W(p,\omega)]\,. \quad (38)$$

$\mathrm{Re}[W(p,\omega)]$ and $\mathrm{Im}[W(p,\omega)]$ are the real and imaginary parts of the function $W(p,\omega)$ which are generated by the substitution

$$\frac{1}{\omega-\omega'\pm i\epsilon}=\mathcal{P}\left(\frac{1}{\omega-\omega'}\right)\mp i\pi\delta(\omega-\omega')\,;$$
$$\mathcal{P}=\text{principal value function}\,,\qquad \delta(x)=\text{delta function}\,. \quad (39)$$

These results are of a quite general nature.[7] The real part of the pole given by the coefficient of the G_1 function gives the renormalized energy of the magnons. The magnon energy E_m is then given by the equation

$$E_m=-\omega=\epsilon(p,\omega)\,. \quad (40)$$

The imaginary part of the pole gives the lifetime τ^{-1} of this single-particle state with energy E_m.

At low temperatures the solution of (40) is clearly

$$E_m=\epsilon(p,\omega=-E_p{}^0)=E_p{}^0-E_p{}^{\mathrm{HF}}-\Sigma(p)=\epsilon(p) \quad (41)$$

with the corresponding lifetime

$$\tau^{-1}(p,\omega=-E_p{}^0)\equiv\tau^{-1}(p)\,. \quad (42)$$

The renormalized magnon energy Eq. (41) is thus composed of three terms. The first is the first-order energy. The second term is generated by the Hartree-Fock terms in (31) and is called the Hartree-Fock energy. It represents a decrease in the energy of the magnon due to its moving independently through an average potential field, and therefore does not represent energy correction due to magnon-magnon interactions.

The last term in (41) represents the energy contribution due to magnon-magnon interactions. This term is the average energy gained by a magnon of momentum p as a result of its correlations with all of the other magnons in the system.

The function $\Sigma(p)$ is discussed in Appendix II and $\tau^{-1}(p)$ is discussed in Sec. V.

There is no justification for the renormalization procedure $G_1{}^0\rightarrow G_1$ within the framework of the approximation characterized by $G_3=0$. We will now try to justify this replacement of $G_1{}^0$ by G_1 as being consistent with the effect of an improved approximation on G_3. A more detailed account of the following is contained in Ref. 6.

Suppose we write out the equation of motion for $G_3(1,2,3,4,5,t)$ defined by Eq. (25). This equation contains inhomogeneous terms coming from the equal-time commutators, terms proportional to G_3 expressing the dynamics of the three reversed spins, and terms proportional to G_4 expressing the interaction of the three reversed spins with other spins in the lattice. We put $G_4=0$ and keep only those terms in G_3 corresponding to noninteracting spin deviations. The solution of the resulting equation is

$$\begin{aligned}G_3(1,2,3,4,5,t)\cong{}&G_1{}^0(1,t)[\langle S_2{}^-S_4{}^+\rangle\langle S_3{}^-S_5{}^+\rangle+\langle S_3{}^-S_4{}^+\rangle\langle S_2{}^-S_5{}^+\rangle]+G_1{}^0(2,t)[\langle S_1{}^-S_4{}^+\rangle\langle S_3{}^-S_5{}^+\rangle\\&+\langle S_3{}^-S_4{}^+\rangle\langle S_1{}^-S_5{}^+\rangle]+G_1{}^0(3,t)[\langle S_1{}^-S_4{}^+\rangle\langle S_2{}^-S_5{}^+\rangle+\langle S_2{}^-S_4{}^+\rangle\langle S_1{}^-S_5{}^+\rangle]\,.\end{aligned}$$

Now replace $G_1{}^0$ by G_1 and utilize the Hartree-Fock expansion of G_2 in terms of G_1 given by Eq. (31) above (with $U=0$). This yields the approximation

$$G_3(1,2,3,4,5,t)\cong\langle S_2{}^-S_4{}^+\rangle G_2(1,3,5,t)+\langle S_1{}^-S_4{}^+\rangle\times G_2(2,3,5,t)+\langle S_3{}^-S_4{}^+\rangle G_2(1,2,5,t)\,.$$

If now this G_3 is substituted in Eq. (24) for G_2, there results a new renormalized coefficient for G_2. The coefficient of G_2 in Eq. (29) is now replaced as follows:

$$(\omega+\mu\mathcal{H}+E_{p_1}{}^0+E_{p_2}{}^0-E_{p_3}{}^0)\rightarrow(\omega+\mu\mathcal{H}+\Gamma_{p_1}+\Gamma_{p_2}-\Gamma_{p_3})$$

with

$$\Gamma_p=E_p{}^0-E_p{}^{\mathrm{HF}}\,,$$

showing that $E_p{}^0$ has been replaced by $E_p{}^0-E_p{}^{\mathrm{HF}}$ in the solution for G_2. Therefore, the replacement of $E_p{}^0$ by E_p in the G_2 equation (I14) seems to be consistent with the effect that the G_3 functions have on this equation. The proof is not complete, because the energy $E_p{}^0-E_p{}^{\mathrm{HF}}$ differs from E_p by the function $W(p,\omega)$ given in Eq. (35). This difference is the magnon-magnon interaction term and was generated by a detailed solution of the G_2 equation. Such a term as $W(p,\omega)$ would presumably enter the renormalized G_2 coefficient if a more detailed representation of G_3 were made in this equation. The explicit demonstration of this remains a program for future work.

IV. CORRELATION FUNCTIONS, MAGNETIZATION, AND SPECIFIC HEAT

The correlation function $\langle S_n{}^-(t)S_0{}^+(0)\rangle$ can be calculated from the knowledge of the Fourier transform of the G_1 function,

$$G_1(j,t)=\frac{1}{2\pi N}\sum_p\int_{-\infty}^{\infty}G_1(p,\omega)e^{-i\omega t}e^{ip\cdot j}d\omega\,. \quad (43)$$

In terms of $G_1(p,\omega)$, Eq. (6) becomes, in the limit $N\rightarrow\infty$,

$$\langle S_n{}^-(t)S_0{}^+(0)\rangle=\lim_{\epsilon\rightarrow0}\frac{iv}{(2\pi)^4}\int d^3p\int_{-\infty}^{\infty}d\omega\,\frac{e^{ip\cdot n}e^{-i\omega t}}{1-e^{-\beta\omega}}[G_1(p,\omega+i\epsilon)-G_1(p,\omega-i\epsilon)]\,. \quad (44)$$

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[7] L. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, Inc., New York, 1962), Chaps. 3 and 4.

The discontinuity of $G_1(p,\omega)$ across the real axis can be obtained from (36). The integration over ω in (44) is performed by treating ω as a complex variable. The contour chosen for $t>0$ $(t<0)$ is one which is closed in the lower (upper) half complex ω plane. In either case the contribution to the integral from the semicircles is zero. The resulting expression is quite complicated, only the leading temperature term is given below:

$$\langle S_n^-(t)S_0^+(0)\rangle=\frac{2\langle S^z\rangle v}{(2\pi)^3}\int\langle n\rangle_p \times e^{i\mathbf{p}\cdot\mathbf{n}}e^{-(\tau-1/2)|t|}e^{i\epsilon(p)t}d^3p+\cdots. \tag{45}$$

Evaluation of $\langle S_n^-(t)S_0^+(0)\rangle$ for $\mathbf{n}=t=0$ gives the relatively simple expression

$$\langle S_0^-S_0^+\rangle=\frac{2\langle S^z\rangle v}{(2\pi)^3}\int\langle n\rangle_p d^3p-\frac{4v^3}{(2\pi)^9}\int\int\int\frac{S_{p-p_1-p_2}[\gamma_{p-p_1}-\gamma_{p_2}]}{(\gamma_p-\gamma_{p_1}-\gamma_{p_2}+\gamma_{p-p_1-p_2})}[\langle n\rangle_p-\langle n\rangle_{p,p_1,p_2}]d^3p_1d^3p_2d^3p$$
$$-\frac{4v^4J^2}{(2\pi)^{12}}\int\int\int\int\frac{S_{p-p_1-p_2}\langle n\rangle_{p,p_1,p_2}[\gamma_{p_1-p'}-\gamma_{p'}][\gamma_{p-p_1}+\gamma_{p-p_2}-\gamma_{p_1}-\gamma_{p_2}]}{[E_{p_1}{}^0+E_{p_2}{}^0-E_p{}^0-E_{p-p_1-p_2}{}^0][E_{p'}{}^0+E_{p'-p_1-p_2}{}^0-E_p{}^0-E_{p-p_1-p_2}{}^0]}d^3p_1d^3p_2d^3p'd^3p, \tag{46}$$

where

$$\langle n\rangle_p=(e^{\beta\epsilon(p)}-1)^{-1}, \tag{47}$$

$$\langle n\rangle_{p,p_1,p_2}=(e^{\beta E_{p_1}{}^0+E_{p_2}{}^0-E_{p-p_1-p_2}{}^0)}-1)^{-1}. \tag{48}$$

The second term in (46) is generated by the term $\delta_{1,0}\delta_{2,0}\langle S_1^-S_3^+\rangle$ in the G_2 equation, which guarantees the exact solution of this equation to be zero if $1=2$, as it should be. By making the substitution $\mathbf{p}_2=\mathbf{p}_a-\mathbf{p}_1-\mathbf{p}_2$, expanding the integrand for small $\mathbf{p}_a$ and $\mathbf{p}$, and using Eq. (30) in the first part of this second term gives

$$\frac{-2v^2}{(2\pi)^6}\langle S_0^-S_0^+\rangle\int\int\langle n_p\rangle\frac{\gamma_{p-p_1}-\gamma_{p_1}}{\gamma_0-\gamma_{p_1}}d^3pd^3p_1. \tag{49}$$

The second part of the second term in (46) is simplified by solving the G_1 equation with $G_2=0$, giving the first-order result

$$G_1{}^0(p,\omega)=-2\langle S^z\rangle/(\omega+E_p{}^0). \tag{50}$$

This result is then substituted into (44) to calculate $\langle S_0^-S_n^+\rangle$ and hence to calculate the first-order approximation for S_p. The result is

$$S_p=2\langle S^z\rangle\langle n_p\rangle^0, \tag{51}$$

with

$$\langle n\rangle_p{}^0=(e^{\beta E_p{}^0}-1)^{-1}. \tag{52}$$

Then

$$S_{p-p_1-p_2}\langle n\rangle_{p,p_1,p_2}=2\langle S^z)$$
$$\times\frac{\langle n\rangle_{p-p_1-p_2}{}^0[1+\langle n\rangle_{p-p_1-p_2}{}^0]\langle n\rangle_{p_1}{}^0\langle n\rangle_{p_2}{}^0}{\langle n\rangle_{p-p_1-p_2}{}^0[1+\langle n\rangle_{p_1}{}^0+\langle n\rangle_{p_2}{}^0]-\langle n\rangle_{p_1}{}^0\langle n\rangle_{p_2}{}^0}. \tag{53}$$

Since $H\neq 0$, this expression becomes (for small H)

$$S_{p-p_1-p_2}\langle n\rangle_{p,p_1,p_2}\cong 2\langle S^z\rangle\langle n\rangle_{p_1}{}^0\langle n\rangle_{p_2}{}^0. \tag{54}$$

Then using (54), the second part of the second term in (46) becomes

$$2\langle S^z\rangle\frac{2v^2}{(2\pi)^-}\int\int\langle n\rangle_{p_1}{}^0\langle n\rangle_{p_2}{}^0d^3p_1d^3p_2$$
$$=\langle S^z\rangle\left[\frac{2v}{(2\pi)_3}\int\langle n\rangle_p{}^0d^3p\right]^2. \tag{55}$$

After using the approximation (51), the last term in (46) becomes

$$\frac{2v^2}{(2\pi)^6}\left[\frac{2\langle S^z\rangle v}{(2\pi)_3}\int\langle n\rangle_p{}^0d^3p\right]$$
$$\times\left[\int\int\langle n\rangle_p{}^0\frac{\gamma_{p-p_1}-\gamma_{p_1}}{\gamma_0-\gamma_{p_1}}d^3pd^3p_1\right]. \tag{56}$$

Substitution of (49), (55), and (56) into (46) gives

$$\langle S_0^-S_0^+\rangle=\frac{2\langle S^z\rangle v}{(2\pi)^3}\int\langle n\rangle_p d^3p$$
$$+\langle S^z\rangle\left[\frac{2v}{(2\pi)^3}\int\langle n\rangle_p{}^0d^3p\right]^2, \tag{57}$$

since (49) and (56) cancel up to order $T^{13/2}$, which is well above the range of validity of this theory.

The magnetization per spin, M, is defined by

$$M=\langle S^z\rangle/S=1-2\langle S_0^-S_0^+\rangle. \tag{58}$$

Substituting (57) into (58) and solving for M gives

$$M=\frac{1}{1+2\eta+[2\eta_0]^2}=1-2\eta+(2\eta)^2-(2\eta_0)^2+\cdots, \tag{59}$$

where

$$\eta_0=\frac{v}{(2\pi)^3}\int\langle n\rangle_p{}^0d^3p, \tag{60}$$

$$\eta=\frac{v}{(2\pi)^3}\int\langle n\rangle_p d^3p. \tag{61}$$

In order to evaluate M the renormalized energies $\epsilon(p)$ must be known. From Eqs. (II25) and (II27),

$$\epsilon(p)=J(\gamma_0-\gamma_p)[1-\eta_1]-(Q-1)J(pa)^2f_0(T),$$

$$\eta_1=\frac{2v}{(2\pi)^3}\int\langle n\rangle_p{}^0(\gamma_0-\gamma_p)d^3p, \tag{63}$$

where the second term in (62) is the leading temperature and momentum term in $\Sigma(p)$.

Equation of the eta functions in powers of T gives

$$\eta_0(\theta)=\zeta(\tfrac{3}{2})\left(\frac{3\theta}{2\pi\gamma_0\nu}\right)^{3/2}+\tfrac{3}{4}\pi\nu\zeta(\tfrac{5}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{5/2}$$
$$+\pi^2\omega_0{}^2\nu^2\zeta(\tfrac{7}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{7/2}+O(\theta)^{9/2}, \tag{64}$$

$$\eta(\theta)=\zeta(\tfrac{3}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu[1+Qf_0(T)]}\right\}^{3/2}+\tfrac{3}{4}\pi\nu\zeta(\tfrac{5}{2})$$
$$\times\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{5/2}+\pi^2\omega_0{}^2\nu^2\zeta(\tfrac{7}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{7/2}+O(\theta^{9/2}) \tag{65}$$
$$=\eta_0(\theta)+3\pi\nu\zeta(\tfrac{3}{2})\zeta(\tfrac{5}{2})Q\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{4}+O(\theta^{9/2}),$$

$$\eta_1(\theta)=2\pi\nu\zeta(\tfrac{5}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{5/2}+O(\theta^{7/2}), \tag{66}$$

with

$$\theta=k_BT/J=1/J\beta. \tag{67}$$

The constants $\omega_0{}^2$, $\zeta(x)$, and ν are given in Appendix III.

The magnetization at low temperatures then becomes

$$M=1-2\zeta(\tfrac{3}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{3/2}-\tfrac{3}{2}\pi\nu\zeta(\tfrac{5}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{5/2}$$
$$-2\pi^2\omega_0{}^2\nu^2\zeta(\tfrac{7}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{7/2}$$
$$-6\pi\nu Q\zeta(\tfrac{3}{2})\zeta(\tfrac{5}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{4}-O(\theta^{9/2}). \tag{68}$$

The value of Q for the simple cubic lattice derived in Appendix II is

$$Q=1+\tfrac{2}{3}\alpha+\tfrac{4}{3}(\Gamma^S/(1-\Gamma^S)), \tag{69}$$

which agrees exactly with Dyson's value. For the other cubic lattices the agreement should also be exact since this was found to be the case for the simple cubic lattice. The values of Q for the cubic lattices are given in Appendix III.

The anomalous T^3 term which is present in the magnetization formula given by first-order theories has been cancelled out in the second-order theory. The cancellation can be seen in the third and fourth terms in (59):

$$(2\eta)^2-(2\eta_0)^2=4\left[\zeta^2(\tfrac{3}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{3}+\tfrac{3}{2}\pi\nu\zeta(\tfrac{3}{2})\zeta(\tfrac{5}{2})\right.$$
$$\left.\times\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{4}+\cdots\right]-4\left[\zeta^2(\tfrac{3}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{3}\right.$$
$$\left.+\tfrac{3}{2}\pi\nu\zeta(\tfrac{3}{2})\zeta(\tfrac{5}{2})\left(\frac{3\theta}{2\pi\gamma_0\nu}\right)^{4}+\cdots\right]. \tag{70}$$

It is also noted that the T^4 terms contributed by these terms exactly cancel. The T^3 term is missing in the second-order expression because of its cancellation by the $\delta_{1,0}\delta_{2,0}\langle S_1{}^-S_3{}^+\rangle$ term in the G_2 equation. Thus G_2 being zero if $1=2$ is a necessary condition for the removal of this anomalous T^3 term.

Specific Heat

The specific heat per site is calculated in the following manner. The total energy of a system of magnons at a temperature T is given by

$$U=\sum_p\langle n\rangle_pE_p{}^0-\tfrac{1}{2}\sum_p\langle n\rangle_p[E_p{}^{\mathrm{HF}}+\Sigma(p)], \tag{71}$$

where the factor of $\frac{1}{2}$ accounts for the double counting of the Hartree-Fock and the magnon-magnon interaction energies, and $\langle n\rangle_p$ is the occupation number for magnons of energy E_p at the temperature T. Equation (71) is valid in the approximation of neglecting the imaginary parts of $G_1(p,\omega)$ and $W(p,\omega)$. These terms will make contributions to the energy of order higher than the θ^5 term to which we restrict the accuracy of this specific-heat calculation.

From Eqs. (62) and (66), Eq. (71) becomes

$$U=J(1-\eta_1)\sum_p\langle n\rangle_p(\gamma_0-\gamma_p)$$
$$-\frac{Q-1}{2}f_0(T)\sum_p\langle n\rangle_p(pa)^2. \tag{72}$$

The average energy per lattice site is then U/N, where N is the number of lattice sites. Expansion of U/N in a power series in T gives

$$\frac{U}{N}=J\left[\pi\gamma_0\nu\zeta(\tfrac{5}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{5/2}+(5/4)\pi^2\nu^2\gamma_0\zeta(\tfrac{7}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{7/2}\right.$$
$$+(7/3)\gamma_0\omega_0{}^2\pi^2\nu^3\zeta(\tfrac{9}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{9/2}$$
$$\left.+4\pi^2\nu^2\gamma_0Q[\zeta(\tfrac{5}{2})]^2\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{5}\right]+O(\theta^{11/2}). \tag{73}$$

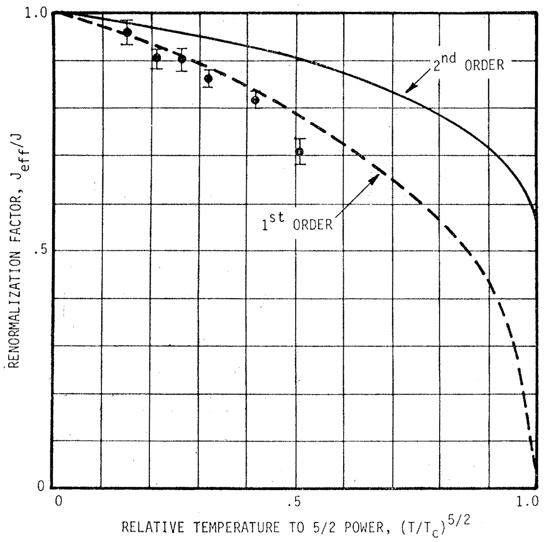

FIG. 1. The renormalization factor for a face-centered cubic lattice. The 1st-order, dashed curve is from Ref. 1. The 2nd-order curve is Eq. (92) of the present work. The experimental data are those of Stringfellow and Torrie in Ref. 8.

Then

$$C=\frac{d}{dT}\left(\frac{U}{N}\right)=k_B\left\{\frac{15}{4}\zeta(\tfrac{5}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{3/2}+\frac{105}{16}\pi\nu\zeta(\tfrac{7}{2})\right.$$
$$\times\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{5/2}+\frac{63}{4}\pi^2\nu^2\omega_0{}^2\zeta(\tfrac{9}{2})\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^{7/2}$$
$$\left.+30\pi\nu Q[\zeta(\tfrac{5}{2})]^2\left\{\frac{3\theta}{2\pi\gamma_0\nu}\right\}^4\right\}+O(\theta^{9/2})\,,\qquad(74)$$

which agrees exactly with Dyson's result.

V. RESULTS AT GENERAL TEMPERATURES, RENORMALIZED MAGNON ENERGIES

The second-order calculation has produced a renormalization of the first-order energy $E_p{}^0$. The second-order energy expression at low temperatures is given by Eq. (II1). This result can also be written as

$$\epsilon(p)=J(\gamma_0-\gamma_p)[1-\Phi]-\Sigma(p)\,,\qquad(75)$$

where

$$\Phi=\frac{2v}{(2\pi)^3}\int\frac{S_p}{2\langle S^z\rangle}(\gamma_0-\gamma_p)d^3p.\qquad(76)$$

The lowest order temperature and momentum term in $\Sigma(p)$, given in Appendix II, can be reproduced by the function

$$\Sigma(p)=J(\,Q-1)(\gamma_0-\gamma_p)\Phi.\qquad(77)$$

Substitution of this result into (75) gives

$$\epsilon(p)=J(\gamma_0-\gamma_p)[1-Q\Phi]\equiv J_{\text{eff}}(\gamma_0-\gamma_p)\,,\qquad(78)$$

$$J_{\text{eff}}/J=1-Q\Phi.\qquad(79)$$

The first-order result for S_p is given by Eq. (51). The second-order theory could be used to calculate S_p for all p, provided one could do the complicated integrals which are functions of p. A compromise between these two methods is to use the Hartree-Fock approximation, given by Eq. (31) with $U(1,2,3,t)=0$, to calculate S_p. It follows that

$$\Phi=\frac{2v}{(2\pi)^3}\int\frac{\gamma_0-\gamma_p}{e^{J\beta(\gamma_0-\gamma_p)(1-\Phi)}-1}d^3p.\qquad(80)$$

The ratio J_{eff}/J can be measured by inelastic neutron diffraction.[8] Figure 1 shows a plot of Eq. (79) with $\Phi(\theta)$ given by (80) for a face-centered cubic lattice, as evaluated on the Georgia Tech Burroughs B5500 computer. A value of $\theta_c=4$ was used to determine θ/θ_c. It should be emphasized here that this choice of θ_c does not in any way influence the values of Φ for a given θ.

Figure 1 also shows the results from experiments on nickel, which is a face-centered cubic lattice with s close to one-half (0.6 holes in the d band), which were reported by Lowde. The results from I are also given.

The experimental J_{eff} falls off more rapidly with temperature than predicted by this theory. The main reason for this is that the nearest-neighbor model discussed here cannot be applied to nickel.[9] This point is discussed in more detail in the next section.

From Fig. 1 it follows that the magnon energy does not go to zero at the Curie point. It is clear that better approximations of S_p calculated in this termination and higher order terminations of the Green's functions will cause the energy near the Curie point to decrease

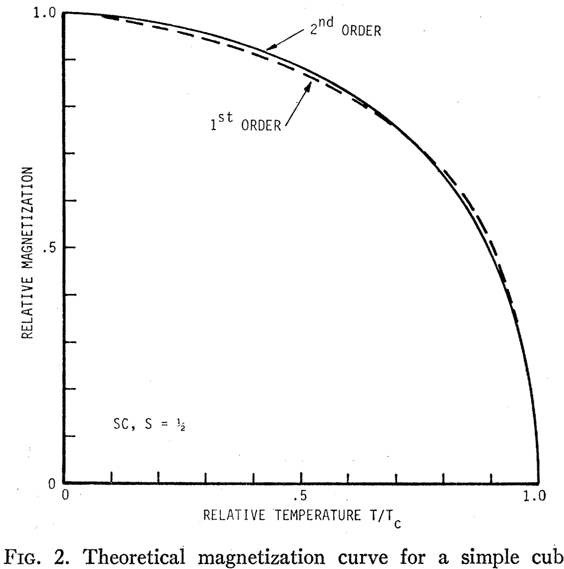

FIG. 2. Theoretical magnetization curve for a simple cubic lattice. The 1st-order, dashed curve is our earlier result from Ref. 1. The present work yields the curve marked 2nd order.

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[8] R. D. Lowde, J. Appl. Phys. **36**, 884 (1965). The experimental data in Fig. 2 are those of M. W. Stringfellow and B. H. Torrie.

[9] B. E. Argyle, S. H. Charap, and E. W. Pugh, Phys. Rev. **132**, 2051 (1963).

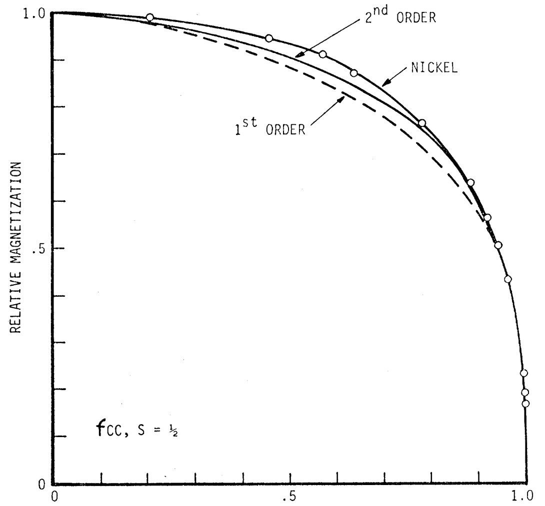

FIG. 3. The magnetization curve for nickel compared with theory. The 1st-order, dashed curve is from Ref. 1; the present work results in the 2nd-order curve.

further. The question of whether or not it will actually go to zero at the Curie point cannot be answered in this termination.

The Magnetization

The magnetization formula (68) for the nearest-neighbor approximation is in exact agreement with Dyson's results to order θ^4. In order to extend these results to higher temperatures only those terms which contribute to the magnetization formula to order θ^4 or less are retained. That is,

$$M=1-2\eta\,, \tag{81}$$

where η is defined by Eq. (61), which is calculated using (79) and (80).

The magnetization given by (81) has been evaluated on a computer and the results for the simple cubic (sc) and face-centered (fcc) cubic lattices are plotted in Figs. 2 and 3, respectively. The simple cubic and body-centered cubic (bcc) curves intersect the (θ/θ_c) axis and continue on for negative values of M, eventually becoming double valued. The face-centered-cubic curve may become double valued before reaching the θ/θ_c axis somewhere in the range $M<0.07$. In order to settle this question an accuracy of about 0.01% is needed in the calculation of Φ for temperatures near θ_c. The values of Φ were calculated to about 1% accuracy. The fact that these curves do not give zero for $\theta>\theta_c$ is due to the approximations used and in the termination $G_3=0$.

The values of θ_c found from (77) are given in Table I below.

These values of θ_c are in close agreement with those given by Rushbrooke[4] from the high-temperature series expansions and are somewhat closer than those predicted by I or by Callen.

The relatively poor agreement with the nickel data in Fig. 3 is due to the fact that the nearest-neighbor model is incapable of fitting the low-temperature magnetization data on nickel.[9] The coefficients of the $T^{3/2}$ and $T^{5/2}$ terms in the magnetization formula depend only on J and the value of J computed from the experimental value of the $T^{3/2}$ coefficient gives the wrong experimental $T^{5/2}$ coefficient. As pointed out in Ref. 9, this difficulty can be solved by assuming a position-dependent J, $J(\mathbf{r})$, and expanding M in terms of the moments of $J(\mathbf{r})$.

Further evidence for the necessity for including longer range interactions than nearest neighbors comes from the ratio of the coefficient N of the $T^{5/2}$ term in the energy expansion to the coefficient C of the $T^{5/2}$ term in the magnetization. This ratio, calculated in the Hartree-Fock approximation, yields $N/C=\frac{4}{3}$. The present theory which accounts for magnon-magnon interactions yields $N/C=\frac{4}{3}Q$. Accounting for interactions of arbitrary range in the Hartree-Fock approximation gives $N/C=\frac{4}{3}(1+A_0)$, where A_0 is a function of the moments of the interaction $J(\mathbf{r})$.[10]

In Ref. 9 N/C is determined to be about 4.1 for nickel. A second estimate comes from Lowde's experiment by fitting his points to a $D=D_0(1-NT^{5/2})$ curve, where the value of C is given in Ref. 9, with a resultant N/C value of about 4. This last number may be too high because the lowest temperature used in Lowde's experiment is nearly 42% of the Curie temperature, and higher order terms in the energy may be comparable to the $T^{5/2}$ term. Nonetheless there appears to be adequate evidence for the necessity of including more than nearest-neighbor interactions, and these will affect our predicted magnetization curve.

Lifetimes

The imaginary part of the renormalized energy given by (38) is interpreted as the lifetime of a single-particle state. The low-temperature expansion of (38) is obtained by using (51) for S_p. After one integration, the leading term is

$$\tau^{-1}(p)=\frac{2Jv^2p^2a^2}{(2\pi)^4}\int_0^\infty\int_0^\pi\int_0^{2\pi}\langle n\rangle_{p'}|\mathbf{p}'-\mathbf{p}| \times|\mathbf{p}'|^2\cos^2\varphi\, d^3\mathbf{p}'\,, \tag{82}$$

where φ is the angle between $\mathbf{p}$ and $\mathbf{p}'$. The leading term

TABLE I. Curie temperatures given by different approximations.

θ_c	Present work	Rushbrooke	I	Callen
sc	1.91	1.68	2.0	2.7
bcc	2.64	2.52	2.9	3.7
fcc	4.0	4.0	4.5	5.6

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[10] W. Marshall (unpublished).

of (82) is then

$$\tau^{-1}(p)=\left(\frac{6}{\gamma_0 v}\right)^3\frac{J\sqrt{\pi}}{16\pi^3}\zeta(\tfrac{5}{2})(pa)^3\theta^{5/2},\quad pa\gg\theta^{1/2}\qquad(83)$$

$$\tau^{-1}(p)=\left(\frac{6}{\gamma_0 v}\right)^3\frac{J}{6\pi^3}\zeta(3)(pa)^2\theta^3,\qquad pa\ll\theta^{1/2},\quad(84)$$

where a is the lattice constant.

Equation (83) agrees with the lifetime calculated from Dyson's[3] mean free path, after Eq. (111) of Ref. 3 has been corrected by replacing $\zeta(\frac{3}{2})$ by $\zeta(\frac{5}{2})$.

VI. CONCLUSIONS

This work shows that it is possible to solve the second-order Green's-function equations defined for the Heisenberg Hamiltonian within an energy renormalization framework, providing in the case of the nearest-neighbor approximation expressions for the magnon-magnon interaction energy and lifetimes for single-particle excited states. These expressions are generated by the G_2 equation and are not introduced into the theory from external arguments.

Because of the agreement of the results obtained in this work with Dyson's results, it is concluded that the Green's-function theory is providing a well-ordered scheme for calculation of the physical properties for the Heisenberg ferromagnet. The second-order theory presented here yields results only slightly different from first-order theory for the temperature dependence of spontaneous magnetization. There is a larger difference in the predictions of the two approximations for the temperature dependence of the effective exchange interaction. Apparently, there is no experimental data for insulating ferromagnets with spin $\frac{1}{2}$ which would allow comparison of effective exchange interactions as given by the two approximations. The case of nickel, for which some experimental information is available, appears to call for including longer range exchange interactions than merely nearest neighbors. From the theory side, it would be useful to have calculations extending the present results to the case of longer range exchange interactions. Also, extension of this second-order calculation to include higher spin values would probably be worthwhile. Finally, it would be desirable of supplement the computer results with analysis in the vicinity of the Curie temperature.

Apparently the results of neutron diffraction experiments determining the effective exchange interactions and the magnon lifetimes as the Curie temperature is approached will provide sensitive tests for this and other refinements of the first-order theory.

ACKNOWLEDGMENTS

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APPENDIX I: CALCULATION OF G_2 FOR NEAREST-NEIGHBOR APPROXIMATION

Equation (29) is solved by letting $N\to\infty$. In this limit p becomes a continuous variable and

$$\frac{1}{N}\sum_p\to\frac{v}{(2\pi)^3}\int d^3p,\qquad(\mathrm{I}1)$$

where the integration is taken over the first Brillouin zone. The symbol $1/v$ denotes the number of particles per unit volume. In this limit (29) can be solved with the aid of Fredholm theory.[11] Using (I1) and making the substitution

$$[\omega+\mu H+J(\gamma_0-\gamma_{p_1}-\gamma_{p_2}+\gamma_{p_3})]G_2(p_1,p_2,p_3,\omega)=F(p_1,p_2,p_3,\omega),\quad(\mathrm{I}2)$$

Eq. (29) becomes

$$F(p_1,p_2,p_3,\omega)-\frac{2Jv}{(2\pi)^3}\int F(p',p_1+p_2-p',p_3,\omega)\times\frac{\gamma_{p_1-p'}-\gamma_{p'}}{\omega+\mu H+J(\gamma_0-\gamma_{p'}-\gamma_{p_1+p_2-p'}+\gamma_{p_3})}d^3p'$$
$$=-[(2\pi)^3/v]S_{p_3}[\delta(p_1+p_3)+\delta(p_2+p_3)]+2S_{p_3},\quad(\mathrm{I}3)$$

where $\delta(x)$ is the Dirac delta function. Let

$$\alpha_\rho(x)=[2Jv/(2\pi)^3][e^{i\mathbf{x}\cdot\rho}-1],\qquad(\mathrm{I}4)$$

$$\beta_\rho(x)=\frac{e^{-i\mathbf{x}\cdot\rho}}{\omega+\mu H+J(\gamma_0-\gamma_x-\gamma_{p_1+p_2-x}+\gamma_{p_3})}.\qquad(\mathrm{I}5)$$

Then with the substitution $\mathbf{p}_1\to\mathbf{x}$, $\mathbf{p}_2\to\mathbf{p}_1+\mathbf{p}_2-\mathbf{x}$, (I3) becomes

$$F(x,p_1+p_2-x,p_3,\omega)-\int F(x',p_1+p_2-x',p_3,\omega)$$
$$\times\sum_\rho\alpha_\rho(x)\beta_\rho(x')d^3x'=-[2(\pi)^3/v]S_{p_3}$$
$$\times[\delta(x+p_3)+\delta(p_1+p_2+p_3-x)]+2S_{p_3}\equiv I(x).\quad(\mathrm{I}6)$$

This is a Fredholm integral equation of the second kind. The solution is obtained by a direct application of

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[11] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publications, Inc., New York, 1953), Chap. 3.

the Fredholm theory. Let

$$C_{\rho,\rho'}=\int\alpha_\rho(x)\beta_{\rho'}(x)d^3x\,, \tag{I7}$$

$$f_\rho=\int I(x)\beta_\rho(x)d^3x\,. \tag{I8}$$

Then the solution of (I6) is

$$F(x,p_1+p_2-x,p_3,\omega)=I(x)+\sum_\rho x_\rho\alpha_\rho(x)\,, \tag{I9}$$

where the x_ρ are solutions of the matrix equation

$$[I-C]X=f\,, \tag{I10}$$

where I is the unit matrix. For these cubic structures C is a $\gamma_0\times\gamma_0$ matrix.

The solution of (I10) can be written in the form

$$x_\rho=D^{-1}\sum_{\rho'}D_{\rho'}{}^{\rho}f_{\rho'}\,,$$

where the f_ρ are given by (I8) and D is the determinant of the matrix $[I-C]$. The $D_{\rho'}{}^{\rho}$ are minors of the matrix $[I-C]$ which arise naturally in the solution of (I10) by Cramer's method. It is assumed that the minors carry the appropriate factor of $(-1)^n$. Then

$$F(x,p_1+p_2-x,p_3,\omega)=I(x)+D^{-1}\sum_\rho\sum_{\rho'}\alpha_\rho(x)D_{\rho'}{}^{\rho}f_{\rho'}\,. \tag{I12}$$

The functions f_ρ are given by (I8):

$$f_\rho=\frac{-g_\rho(p_3,p_1+p_2+p_3)}{\omega+E_{p_3}{}^0}+h_\rho(p_1+p_2,p_3,\omega)\,;$$

$$\frac{v}{(2\pi)^3}g_\rho(p_3,p_1+p_2+p_3)=S_{p3}[e^{ip_3\cdot\rho}+e^{-i(\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3)\cdot\rho}]\,,$$

$$h_\rho(p_1+p_2,p_3,\omega)=2S_{p3}\int\times\frac{e^{-i\mathbf{p}'\cdot\rho}}{\omega+E_{p'}{}^0+E_{p1+p2-p'}{}^0-E_{p-p1-p2}{}^0}d^3p'\,, \tag{I13}$$

$$E_p{}^0=J(\gamma_0-\gamma_p)+\mu H$$

where $E_p{}^0$ is the first-order magnon energy.

Substitution of (I13) into (I12) gives

$$F(x,p_1+p_2-x,p_3,w)\,.$$

Then using (I3) and (I2) one obtains the $G_2(p_1,p_2,p_3,w)$ solution. Evaluation of this result for $p_3=p-p_1-p_2$ gives

$$\begin{aligned}G_2(p_1,p_2,p-p_1-p_2,\omega)=&\left\{\frac{(2\pi)^3S_{p-p1-p2}}{2\langle S^z\rangle v}[\delta(p-p_1)+\delta(p-p_2)]+\frac{2JS_{p-p1-p2}}{2\langle S^z\rangle}\left[\frac{\gamma_{p-p1}+\gamma_{p-p2}-\gamma_p-\gamma_{p-p1-p2}}{\omega+E_{p1}{}^0+E_{p2}{}^0-E_{p-p1-p2}{}^0}\right]\right.\\&\left.+\frac{2vJ}{2\langle S^z\rangle(2\pi)^3}\sum_\rho\sum_{\rho'}\int\frac{D_{\rho'}{}^{\rho}\alpha_\rho(p')g_{\rho'}(p-p_1-p_2,p)[\gamma_{p1-p'}-\gamma_{p'}]d^3p'}{D[\omega+E_{p1}{}^0+E_{p2}{}^0-E_{p-p1-p2}{}^0][\omega+E_{p'}{}^0+E_{p1+p2-p'}{}^0-E_{p-p1-p2}{}^0]}\right\}\left\{\frac{-2\langle S^z\rangle}{\omega+E_p{}^0}\right\}\\&+\frac{2S_{p-p1-p2}}{\omega+E_{p1}{}^0+E_{p2}{}^0-E_{p-p1-p2}{}^0}+\frac{4JvS_{p-p1-p2}}{(2\pi)^3}\int\frac{\gamma_{p1-p'}-\gamma_{p'}d^3p'}{[\omega+E_{p1}{}^0+E_{p2}{}^0-E_{p-p1-p2}{}^0][\omega+E_{p'}{}^0+E_{p1+p2-p'}{}^0-E_{p-p1-p2}{}^0]}\\&+\frac{2Jv}{(2\pi)^3}\sum_\rho\sum_{\rho'}\int\frac{D_{\rho'}{}^{\rho}\alpha_\rho(p')h_{\rho'}(p_1+p_2,p-p_1-p_2,\omega)[\gamma_{p1-p'}-\gamma_{p'}]d^3p'}{D[\omega+E_{p1}{}^0+E_{p2}{}^0-E_{p-p1-p2}{}^0][\omega+E_{p'}{}^0+E_{p'-p1-p2}{}^0-E_{p-p1-p2}{}^0]}\,.\end{aligned} \tag{I14}$$

The above equation is written in a form to suggest the method of renormalization. The substitution [Eq. (50)]

$$-2\langle S^z\rangle/(\omega+E_p{}^0)=G_1{}^0(p,\omega)\rightarrow G_1(p,\omega) \tag{I15}$$

is now made in (I14). A discussion of this replacement is contained at the end of Sec. III.

APPENDIX II: THE RENORMALIZED MAGNON ENERGY

The renormalized energy $\epsilon(p)$ is a sum of three terms:

$$\epsilon(p)=E_p{}^0-E_p{}^{\mathrm{HF}}-\sum(p)\,. \tag{II1}$$

The interaction energy $\sum(p)$ can be shown to reduce to the form

$$\begin{aligned}\sum(p)=&\frac{2v^2J^2}{(2\pi)^6}\int\int\frac{S_{p-p1-p2}[\gamma_{p1}+\gamma_{p2}-\gamma_{p-p1}-\gamma_{p-p2}]^2}{2\langle S^z\rangle[E_{p1}{}^0+E_{p2}{}^0-E_p{}^0-E_{p-p1-p2}{}^0]}d^3p_1d^3p_2\\&+\frac{2v^3J^2}{(2\pi)^9}\sum_\rho\sum_{\rho'}\int\int\int\frac{D_{\rho'}{}^{\rho}\alpha_\rho(p')g_{\rho'}(p-p_1-p_2,p)[\gamma_{p-p1}+\gamma_{p-p2}-\gamma_{p1}-\gamma_{p1}-\gamma_{p2}][\gamma_{p1-p'}-\gamma_{p'}]d^3p_1d^3p_2d^3p'}{2\langle S^z\rangle D[E_{p1}{}^0+E_{p2}{}^0-E_p{}^0-E_{p-p1-p2}{}^0][E_{p'}{}^0+E_{p1+p2-p'}{}^0-E_p{}^0-E_{p-p1-p2}{}^0]}\,.\end{aligned}$$

The first term in this expression is the result which can be derived from second-order perturbation theory. It is obvious that $\sum(p)$ is even in p and $\sum(p=0)=0$. Thus the first possible nonzero term in an expansion of $\sum(p)$ in powers of p is of the form $\sum(p)=Ap^2$. This approximation can easily be obtained for the simple cubic lattice. Introduction of the variable

$$\mathbf{x}=\mathbf{p}_1+\mathbf{p}_2-\mathbf{p} \tag{II3}$$

for p_2, expanding the integrands at (II2) for small x and p, and using Eq. (51) for S_p gives the leading momentum and temperature term for $\sum(p)$ as

$$\sum(p)=J\sum_{\rho}\sum_{\rho'} d_{\rho\rho'}(\mathbf{p}\cdot\boldsymbol{\rho})(\mathbf{p}\cdot\boldsymbol{\rho}')f_{\rho\rho'}(T)+JR\sum_{\rho 1}\sum_{\rho 2}\sum_{\rho 3} d_{\rho 1,-\rho 3}e_{\rho 2,\rho 3}(\mathbf{p}\cdot\boldsymbol{\rho}_1)(\mathbf{p}\cdot\boldsymbol{\rho}_2)f_{\rho 1,\rho 2}(T)\,, \tag{II4}$$

where

$$d_{\rho,\rho'}=\frac{v}{(2\pi)^3}\int\frac{\cos\mathbf{p}_1\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}')}{\gamma_0-\gamma_{p1}}d^3p_1\,, \tag{II5}$$

$$e_{\rho 1,\rho 2}=\frac{v}{(2\pi)^3}\int\frac{e^{i\mathbf{p}\cdot\rho 1}[e^{i\mathbf{p}\cdot\rho 2}-1]}{\gamma_0-\gamma_p}d^3p\,, \tag{II6}$$

and R is given by

$$R=(D_1+D_3-2D_2)/D_0\,, \tag{II7}$$

$$D_0=\begin{vmatrix} a & b & b & c & b & b\\ b & a & b & b & c & b\\ b & b & a & b & b & c\\ c & b & b & a & b & b\\ b & c & b & b & a & b\\ b & b & c & b & b & a\end{vmatrix}\qquad D_1=\begin{vmatrix} a & b & b & c & b\\ b & a & b & b & c\\ b & b & a & b & b\\ c & b & b & a & b\\ b & c & b & b & a\end{vmatrix}$$

$$D_2=-\begin{vmatrix} b & b & c & b & b\\ b & a & b & b & c\\ b & b & a & b & b\\ c & b & b & a & b\\ b & c & b & b & a\end{vmatrix}\qquad D_3=-\begin{vmatrix} b & b & c & b & b\\ a & b & b & c & b\\ b & a & b & b & c\\ c & b & b & a & b\\ b & c & b & b & a\end{vmatrix} \tag{II8}$$

$$a=1-\frac{v}{(2\pi)^3}\int\frac{1-\cos\mathbf{p}\cdot\boldsymbol{\rho}}{\gamma_0-\gamma_p}d^3p=1-\frac{1}{\gamma_0}\,, \tag{II9}$$

$$b=-\frac{v}{(2\pi)^3}\int\frac{\cos\mathbf{p}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}')-\cos\mathbf{p}\cdot\boldsymbol{\rho}'}{\gamma_0-\gamma_p}d^3p;\quad \boldsymbol{\rho}\neq\boldsymbol{\rho}',-\boldsymbol{\rho}'\,, \tag{II10}$$

$$c=-\frac{v}{(2\pi)^3}\int\frac{\cos 2\mathbf{p}\cdot\boldsymbol{\rho}-\cos\mathbf{p}\cdot\boldsymbol{\rho}}{\gamma_0-\gamma_p}d^3p\,. \tag{II11}$$

The temperature-dependent term $f_{\rho 1,\rho 2}(T)$ in (II4) is the leading temperature term of the integral

$$\frac{v}{(2\pi)^3}\int\langle n\rangle_k(\mathbf{k}\cdot\boldsymbol{\rho}_1)(\mathbf{k}\cdot\boldsymbol{\rho}_2)d^3\mathbf{k} =\frac{4\pi}{3}\boldsymbol{\rho}_1\cdot\boldsymbol{\rho}_2\frac{v}{(2\pi)^3}\int_0^\infty\langle n\rangle_k k^4dk\,. \tag{II12}$$

Define $f_0(T)$ by

$$f_{\rho 1,\rho 2}(T)=\frac{\boldsymbol{\rho}_1\cdot\boldsymbol{\rho}_2}{\rho^2}f_0(T)\,, \tag{II13}$$

then

$$f_0(T)=\frac{\zeta(\frac{5}{2})}{16\pi^{3/2}}\theta^{5/2},\quad \theta=k_BT/J\,. \tag{II14}$$

Because of the orthogonality of the ρ_i for the simple cubic lattice, (II4) can be reduced to a relatively simple form:

$$\Sigma(p)=J(pa)^2f_0(T)\times\{2[d_0+d_1]+4Re_0[d_0+d_1-2d_2]\}\,, \tag{II15}$$

where

$$d_0=d_{\rho,\rho};\quad d_1=d_{\rho 1,-\rho};\quad d_2=d_{\rho,\rho'}\,,\quad \text{for}\quad \boldsymbol{\rho}\neq\boldsymbol{\rho}',-\boldsymbol{\rho}'$$

$$e_0=\frac{v}{(2\pi)^3}\int\frac{(\cos\mathbf{p}\cdot\boldsymbol{\rho})(\cos\mathbf{p}\cdot\boldsymbol{\rho}-1)}{\gamma_0-\gamma_p}d^3p\,. \tag{II16}$$

In terms of Dyson's

$$\Gamma^S=-\frac{6v}{(2\pi)^3}\int\frac{(\cos\mathbf{p}\cdot\boldsymbol{\varrho}_1)(\cos\mathbf{p}\cdot\boldsymbol{\varrho}_2-1)d^3p}{\gamma_0-\gamma_p}, \qquad \boldsymbol{\varrho}_1\neq\boldsymbol{\varrho}_2,-\boldsymbol{\varrho}_2 \tag{II17}$$

and

$$\alpha=\frac{v}{(2\pi)^3}\int\frac{\gamma_p}{\gamma_0-\gamma_p}d^3p, \tag{II18}$$

the above constants become

$$\begin{aligned} e_0&=\tfrac{1}{3}\Gamma^S, & d_1&=\tfrac{2}{3}\Gamma^S+\tfrac{1}{6}(\alpha-1), \\ d_0&=\tfrac{1}{6}(\alpha+1), & d_2&=\tfrac{1}{6}(\alpha-\Gamma^S). \end{aligned} \tag{II19}$$

Then

$$\Sigma(p)=J(pa)^2f_0(T)\{\tfrac{2}{3}\alpha+\tfrac{4}{3}\Gamma^S+\tfrac{4}{3}(\Gamma^S)^2R\}. \tag{II20}$$

The constant R is evaluated in terms of Γ^S by using the identities

$$a=\tfrac{5}{6},\ b=\tfrac{1}{6}\Gamma^s,\ c=\tfrac{1}{6}-\tfrac{2}{3}\Gamma^s, \tag{II21}$$

giving

$$R=\frac{D_1+D_3-2D_2}{D_0}=\frac{\{\frac{2}{3}[1+\Gamma^S]\}^3(1-\Gamma^S)}{\{\frac{2}{3}[1+\Gamma^S]\}^3\{1-\Gamma^S\}^2}=\frac{1}{1-\Gamma^S}. \tag{II22}$$

Then

$$\Sigma(p)=J(pa)^2f_0(T)\{\ Q-1\} \tag{II23}$$

with

$$Q=1+\tfrac{2}{3}\alpha+\tfrac{4}{3}[\Gamma^S/(1-\Gamma^S)]. \tag{II24}$$

The Hartree-Fock energy can be evaluated in a similar manner, giving

$$\begin{aligned} E_p^{\mathrm{HF}}&\cong\frac{2v}{(2\pi)^3}\int\langle n\rangle_p{}^0[\gamma_0-\gamma_p-\gamma_{p'}+\gamma_{p-p'}]d^3p' \\ &=J(pa)^2f_0(T)+\cdots. \end{aligned} \tag{II25}$$

Therefore the leading temperature and momentum term in the renormalized energy is

$$\epsilon(p)=J(pa)^2\{1-Qf_0(T)\}. \tag{II26}$$

It can be shown that Eqs. (II25) and (II26) are correct for the other cubic lattices with $f_0(T)$ defined by(II12) and (II13) for those lattices. The constant Q is much harder to determine for the fcc and bcc lattices because of the nonorthogonality of the p_i and the larger rank of the determinants involved. Thus for all the cubic lattices

$$\Sigma(p)=J(pa)^2f_0(T)\{Q-1\}+\cdots \tag{II27}$$

with

$$f_0(T)=2\pi\nu\zeta(\tfrac{5}{2})\left\{\frac{3\theta}{2\pi\gamma_0}\right\}^{5/2}. \tag{II28}$$

The constants ν are given in Appendix III, and Q is given by (II24) for the simple cubic lattice.

APPENDIX III: VALUES OF CONSTANTS USED IN THE TEXT

$$\begin{array}{rl} \nu=1 & \mathrm{sc} \\ 2^{1/3} & \mathrm{fcc} \\ 3\times2^{-4/3} & \mathrm{bcc} \end{array} \tag{III1}$$

$$\begin{array}{rl} \omega_0{}^2=33/32 & \mathrm{sc} \\ 15/16 & \mathrm{fcc} \\ 281/288 & \mathrm{bcc} \end{array} \tag{III2}$$

$$\begin{array}{rl} Q=1.68 & \mathrm{sc} \\ 1.35 & \mathrm{fcc} \\ 1.45 & \mathrm{bcc} \end{array} \tag{III3}$$

The Riemann zeta functions have the values

$$\zeta(\tfrac{3}{2})=2.612, \tag{III4}$$

$$\zeta(\tfrac{5}{2})=1.341, \tag{III5}$$

$$\zeta(\tfrac{7}{2})=1.127. \tag{III6}$$