Nonlinear Spin-Wave Theory for Antiferromagnets*

S. H. Liu
Institute for Atomic Research and Department of Physics, Iowa State University, Ames, Iowa
(Received 27 September 1965)

The spin-wave interaction in simple antiferromagnets is studied at higher temperatures by a method similar to that of Bloch for ferromagnets. It is shown that the energy spectrum, the sublattice magnetization, and the internal energy of the system depend on a renormalization parameter $\alpha(T)$. This parameter satisfies an implicit equation from which its dependence on the temperature may be determined. It is found that the equation has a solution only up to a temperature $T_{\max}$ which is within a few percent of the theoretical values of the Néel temperature. At very low temperatures the theory reduces to the Oguchi theory after all quantities are expanded in powers of the temperature. The parallel and perpendicular susceptibilities are also calculated.

I. INTRODUCTION

THE correct theory for the spin-wave interaction in ferromagnets at low temperatures was first worked out by Dyson.[1] He showed that, by a suitable transformation of the operators, the spin Hamiltonian may be cast into an ideal boson Hamiltonian with quartic interaction terms. A perturbative treatment of the quartic terms leads to the now famous T^4 term in the magnetization. In a bold attempt, Bloch[2] truncated the Dyson Hamiltonian and found a solution of the new Hamiltonian at elevated temperatures. A remarkable result of this theory is that a solution is only possible up to a certain maximum temperature which compares rather well with the other estimations of the Curie temperature. At very low temperatures the results of this calculation agree with the Dyson theory. Although the theory does not seem to apply near the Curie point, it may not be a bad extrapolation theory to rather high temperatures.

We sought to extend the Bloch theory to simple antiferromagnets. As in the case of ferromagnets, one can find a nonunitary transformation[3,4] which transforms the spin Hamiltonian into an ideal boson Hamiltonian containing quartic interaction terms. This Hamiltonian is then solved within the random phase approximation by using a formalism similar to the Gorkov theory of superconductivity.[5] The result is shown to be the exact analog of Bloch's theory. The maximum temperature at which the equation for the renormalization parameter has a solution is within a few percent of other theoretical values of the Néel temperature. At very low temperatures where all quantities are expanded in powers of the temperature, the results agree with the Oguchi theory of antiferromagnetic spin waves.[6]

* Work was performed in the Ames Laboratory of the U. S. Atomic Energy Commission, Contribution No. 1794. Part of this work was done at the IBM Watson Research Center, Yorktown Heights, New York.
[1] F. J. Dyson, Phys. Rev. **102**, 1217 (1956); **102**, 1230 (1956).
[2] M. Bloch, Phys. Rev. Letters **9**, 286 (1962).
[3] S. V. Maleev, Zh. Eksperim. i Teor. Fiz. **33**, 1010 (1957) [English transl.: Soviet Phys.—JETP **6**, 776 (1958)].
[4] R. A. Tahir-Kheli and D. ter Haar, Phys. Rev. **127**, 95 (1962).
[5] L. P. Gorkov, Zh. Eksperim. i Teor. Fiz. **34**, 735 (1958) [English transl.: Soviet Phys.—JETP **7**, 505 (1958)].
[6] T. Oguchi, Phys. Rev. **117**, 117 (1960).

II. THEORY

We take for our model a cubic, two-sublattice antiferromagnet with nearest-neighbor interaction. The Hamiltonian has the form

$$H=J\sum_i\sum_\delta \mathbf{S}_{1i}\cdot\mathbf{S}_{2,i+\delta}+J\sum_j\sum_\delta \mathbf{S}_{1,j+\delta}\cdot\mathbf{S}_{2j}, \quad (1)$$

where the indices 1, 2 refer to the two sublattices; i, j denote the lattice sites; and the index for the nearest neighbor of i is $i+\delta$. It is assumed that the spontaneous magnetization of the sublattice 1 is in the $-z$ direction and that of the sublattice 2 in the $+z$ direction. We make the following transformation to ideal boson operators[3,4]:

$$\begin{aligned}
&S_{1i}^-=(2S)^{1/2}[b_{1i}-(2S)^{-1}b_{1i}^*b_{1i}b_{1i}],\\
&S_{1i}^+=(2S)^{1/2}b_{1i}^*,\\
&S_{1i}^z=-S+b_{1i}^*b_{1i},\\
&S_{2j}^-=(2S)^{1/2}[b_{2j}^*-(2S)^{-1}b_{2j}^*b_{2j}^*b_{2j}],\\
&S_{2j}^+=(2S)^{1/2}b_{2j},\\
&S_{2j}^z=S-b_{2j}^*b_{2j}.
\end{aligned} \quad (2)$$

It is easy to show that all the commutation relations between the various spin operators are preserved but the Hermitian conjugate relation between S^+ and S^- is no longer valid. It is also clear that the above transformation introduces nonphysical states because the occupation numbers of the harmonic oscillators may be larger than $2S$. This alters the kinetic interaction between the spin waves and makes the theory inapplicable near the critical temperature. The operators S^+ connect the physical states to the nonphysical states while the operators S^- do not.

Next, we introduce the spin-wave operators

$$\begin{aligned}
b_{1i}&=(2/N)^{1/2}\sum_{\mathbf{k}} c_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{R}_{1i}},\\
b_{2j}&=(2/N)^{1/2}\sum_{\mathbf{k}} d_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{R}_{2j}},
\end{aligned} \quad (3)$$

and their Hermitian conjugates, where $\mathbf{R}_{1i}$ is the position of the ith site of sublattice 1 and similarly for $\mathbf{R}_{2j}$. The periodic boundary condition requires

$$(k_x,k_y,k_z)=(l\pi/L,m\pi/L,n\pi/L),$$

where l, m, and n are integers and L is the number of lattice sites in a linear dimension of each sublattice (assumed to be cubic). In terms of these new operators, the Hamiltonian becomes

$$H=-NJzS^2+2JzS\sum_{\mathbf{k}}[c_{\mathbf{k}}^*c_{\mathbf{k}}+d_{\mathbf{k}}^*d_{\mathbf{k}}+\gamma(\mathbf{k})c_{\mathbf{k}}^*d_{\mathbf{k}}^*+\gamma(\mathbf{k})c_{\mathbf{k}}d_{\mathbf{k}}]$$
$$-JzN^{-1}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}[4\gamma(\mathbf{k}-\mathbf{k}')c_{\mathbf{k}}^*c_{\mathbf{k}'}d_{\mathbf{k}+\mathbf{q}}^*d_{\mathbf{k}'+\mathbf{q}}+\gamma(\mathbf{k}+\mathbf{q})c_{\mathbf{k}'}{}^*c_{\mathbf{k}'+\mathbf{q}}d_{\mathbf{k}+\mathbf{q}}+\gamma(\mathbf{k}+\mathbf{q})c_{\mathbf{k}'+\mathbf{q}}{}^*c_{\mathbf{k}}^*c_{\mathbf{k}'}d_{\mathbf{k}+\mathbf{q}}^*$$
$$+\gamma(\mathbf{k})c_{\mathbf{k}}d_{\mathbf{k}'}{}^*d_{\mathbf{k}+\mathbf{q}}d_{\mathbf{k}'-\mathbf{q}}+\gamma(\mathbf{k})c_{\mathbf{k}}{}^*d_{\mathbf{k}+\mathbf{q}}{}^*d_{\mathbf{k}'-\mathbf{q}}{}^*d_{\mathbf{k}'}], \quad (4)$$

where N is the total number of lattice sites, z is the number of nearest neighbors, and

$$\gamma(\mathbf{k})=z^{-1}\sum_{\delta}e^{i\mathbf{k}\cdot\delta}, \quad (5)$$

where δ is a vector connecting nearest neighbors.

We define the following matrix Green's function:

$$\hat{G}(\mathbf{k},\tau)=\begin{pmatrix}G_{11}(\mathbf{k},\tau) & G_{12}(\mathbf{k},\tau)\\ G_{21}(\mathbf{k},\tau) & G_{22}(\mathbf{k},\tau)\end{pmatrix}, \quad (6)$$

where

$$\begin{aligned}G_{11}(\mathbf{k},\tau)&=\langle Tc_{\mathbf{k}}(\tau)c_{\mathbf{k}}{}^*(0)\rangle,\\ G_{12}(\mathbf{k},\tau)&=\langle Tc_{\mathbf{k}}(\tau)d_{\mathbf{k}}(0)\rangle,\\ G_{21}(\mathbf{k},\tau)&=\langle Td_{\mathbf{k}}{}^*(\tau)c_{\mathbf{k}}{}^*(0)\rangle,\\ G_{22}(\mathbf{k},\tau)&=\langle Td_{\mathbf{k}}{}^*(\tau)d_{\mathbf{k}}(0)\rangle.\end{aligned} \quad (7)$$

The operator T is the chronological operator for the imaginary time τ, the Heisenberg operator is defined as

$$A(\tau)=e^{\tau H}Ae^{-\tau H}, \quad (8)$$

and the thermal average is defined as

$$\langle B\rangle=\mathrm{tr}(e^{-\beta H}B)/\mathrm{tr}(e^{-\beta H}), \quad (9)$$

$\beta=(kT)^{-1}$. The Green's function can be Fourier analyzed:

$$\hat{G}(\mathbf{k},\tau)=(1/\beta)\sum_n\hat{G}(\mathbf{k},\omega_n)e^{-i\omega_n\tau}, \quad (10)$$

where $\omega_n=2n\pi/\beta$ and n is an integer. It is rather easy to show that

$$\begin{aligned}G_{11}(\mathbf{k},\omega_n)&=G_{22}(\mathbf{k},-\omega_n),\\ G_{12}{}^*(\mathbf{k},\omega_n)&=G_{21}(\mathbf{k},\omega_n).\end{aligned} \quad (11)$$

There are at least two ways to calculate the matrix Green's function. One way is to treat the quartic terms in Eq. (4) as perturbation and use the diagrammatic method; another way is the equation-of-motion method with the random phase or decoupling approximation. We choose to present the latter method because it is simpler in the lowest order calculation. In higher orders the diagrammatic method is more systematic.

The equation of motion for $\hat{G}$ is easily found to be

$$\frac{d}{d\tau}\hat{G}(\mathbf{k},\tau)=\delta(\tau)\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}+\begin{pmatrix}\langle T[H,c_{\mathbf{k}}(\tau)]c_{\mathbf{k}}{}^*(0)\rangle & \langle T[H,c_{\mathbf{k}}(\tau)]d_{\mathbf{k}}(0)\rangle\\ \langle T[H,d_{\mathbf{k}}{}^*(\tau)]c_{\mathbf{k}}{}^*(0)\rangle & \langle T[H,d_{\mathbf{k}}{}^*(\tau)]d_{\mathbf{k}}(0)\rangle\end{pmatrix}. \quad (12)$$

Working out the commutators, we find

$$\frac{d}{d\tau}G_{11}(\mathbf{k},\tau)=\delta(\tau)-h_e[G_{11}(\mathbf{k},\tau)+\gamma(\mathbf{k})G_{21}(\mathbf{k},\tau)]+2h_e(NS)^{-1}\sum_{\mathbf{k}'\mathbf{q}}\gamma(\mathbf{k}-\mathbf{k}')\langle Tc_{\mathbf{k}'}(\tau)d_{\mathbf{k}+\mathbf{q}}{}^*(\tau)d_{\mathbf{k}'+\mathbf{q}}(\tau)c_{\mathbf{k}}{}^*(0)\rangle$$
$$+h_e(2NS)^{-1}\sum_{\mathbf{k}'\mathbf{q}}\gamma(\mathbf{k}'+\mathbf{q})\langle Tc_{\mathbf{k}'}(\tau)c_{\mathbf{k}+\mathbf{q}}(\tau)d_{\mathbf{k}'+\mathbf{q}}(\tau)c_{\mathbf{k}}{}^*(0)\rangle+h_e(NS)^{-1}\sum_{\mathbf{k}'\mathbf{q}}\gamma(\mathbf{k}+\mathbf{q})\langle Tc_{\mathbf{k}'+\mathbf{q}}{}^*(\tau)c_{\mathbf{k}'}(\tau)d_{\mathbf{k}+\mathbf{q}}{}^*(\tau)c_{\mathbf{k}}{}^*(0)\rangle$$
$$+h_e(2NS)^{-1}\sum_{\mathbf{k}'\mathbf{q}}\gamma(\mathbf{k})\langle Td_{\mathbf{k}+\mathbf{q}}{}^*(\tau)d_{\mathbf{k}'-\mathbf{q}}{}^*(\tau)d_{\mathbf{k}'}(\tau)c_{\mathbf{k}}{}^*(0)\rangle, \quad (13)$$

and similar expressions for the other components. We use a shorthand notation h_e for the exchange field $2JzS$. At this point we make decoupling approximation to the higher order Green's functions, e.g.,

$$\langle Tc_{\mathbf{k}'}(\tau)d_{\mathbf{k}+\mathbf{q}}{}^*(\tau)d_{\mathbf{k}'+\mathbf{q}}(\tau)c_{\mathbf{k}}{}^*(0)\rangle$$
$$\cong\delta_{\mathbf{k}\mathbf{k}'}G_{11}(\mathbf{k},\tau)\langle d_{\mathbf{k}+\mathbf{q}}{}^*d_{\mathbf{k}+\mathbf{q}}\rangle+\delta_{\mathbf{q}0}G_{21}(\mathbf{k},\tau)\langle c_{\mathbf{k}'}d_{\mathbf{k}'}\rangle,$$
$$\langle Tc_{\mathbf{k}'+\mathbf{q}}{}^*(\tau)c_{\mathbf{k}'}(\tau)d_{\mathbf{k}+\mathbf{q}}{}^*(\tau)c_{\mathbf{k}}{}^*(0)\rangle$$
$$\cong\delta_{\mathbf{k}\mathbf{k}'}G_{11}(\mathbf{k},\tau)\langle c_{\mathbf{k}+\mathbf{q}}{}^*d_{\mathbf{k}+\mathbf{q}}{}^*\rangle+\delta_{\mathbf{q}0}G_{21}(\mathbf{k},\tau)\langle c_{\mathbf{k}'}{}^*c_{\mathbf{k}'}\rangle,$$

etc. The complete symmetry between the two sublattices implies

$$\langle c_{\mathbf{k}}{}^*c_{\mathbf{k}}\rangle=\langle d_{\mathbf{k}}{}^*d_{\mathbf{k}}\rangle=n_{\mathbf{k}},\quad \langle c_{\mathbf{k}}d_{\mathbf{k}}\rangle=\langle d_{\mathbf{k}}{}^*c_{\mathbf{k}}{}^*\rangle=\xi_{\mathbf{k}}. \quad (14)$$

Then the equation for $\hat{G}$ may be written as

$$\frac{d}{d\tau}\hat{G}(\mathbf{k},\tau)=\delta(\tau)\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$
$$-h_e(1+\alpha)\begin{pmatrix}1 & \gamma(\mathbf{k})\\ -\gamma(\mathbf{k}) & -1\end{pmatrix}\hat{G}(\mathbf{k},\tau), \quad (15)$$

where

$$\alpha=-2(NS)^{-1}\sum_{\mathbf{q}}[n_{\mathbf{q}}+\gamma(\mathbf{q})\xi_{\mathbf{q}}]. \quad (16)$$

The solution of this equation is, in terms of the Fourier

transforms,

$$\hat{G}(\mathbf{k},\omega_n)=\frac{1}{\omega_n^2+\omega_k^2}\begin{pmatrix} h_e(1+\alpha)+i\omega_n & -h_e\gamma(\mathbf{k})(1+\alpha) \\ -h_e\gamma(\mathbf{k})(1+\alpha) & h_e(1+\alpha)-i\omega_n \end{pmatrix}, \tag{17}$$

where

$$\omega_k=h_e(1+\alpha)[1-\gamma^2(\mathbf{k})]^{1/2}. \tag{18}$$

By definition, Eq. (7),

$$\begin{aligned} n_k&=(1/\beta)\textstyle\sum_n G_{11}(\mathbf{k},\omega_n)e^{i\omega_n\delta} \\ &=\tfrac{1}{2}[1-\gamma^2(\mathbf{k})]^{-1/2}\coth\tfrac{1}{2}\beta\omega_k-\tfrac{1}{2}, \\ \xi_k&=(1/\beta)\textstyle\sum_n G_{12}(\mathbf{k},\omega_n)e^{i\omega_n\delta} \\ &=-\tfrac{1}{2}\gamma(\mathbf{k})[1-\gamma^2(\mathbf{k})]^{-1/2}\coth\tfrac{1}{2}\beta\omega_k, \\ \delta&=0^+. \end{aligned} \tag{19}$$

Substituing into Eq. (16), we find

$$\alpha=(2S)^{-1}\{1-2N^{-1}\textstyle\sum_k[1-\gamma^2(\mathbf{k})]^{1/2}\coth\tfrac{1}{2}\beta\omega_k\}. \tag{20}$$

The solution of this equation gives α as a function of the temperature.

The internal energy may be calculated in the same approximation. By definition, $E=\langle H\rangle$. If we evaluate the thermal average of the quartic terms in the Hamiltonian by the decoupling approximation, we find, after a lengthy calculation,

$$E=-\tfrac{1}{2}NSh_e(1+\alpha)^2. \tag{21}$$

The sublattice magnetization per spin may be found in an analogous way. The result is

$$m=S+\tfrac{1}{2}-N^{-1}\textstyle\sum_k[1-\gamma^2(\mathbf{k})]^{-1/2}\coth\tfrac{1}{2}\beta\omega_k. \tag{22}$$

III. LOW-TEMPERATURE LIMIT

At absolute zero,

$$\alpha_0=(2S)^{-1}\{1-2N^{-1}\textstyle\sum_k[1-\gamma^2(\mathbf{k})]^{1/2}\}=c/2S. \tag{23}$$

The ground-state energy and magnetization are

$$\begin{aligned} E_0&=-\tfrac{1}{2}NSh_e(1+c/2S)^2, \\ m_0&=S-N^{-1}\textstyle\sum_k\{[1-\gamma^2(\mathbf{k})]^{-1/2}-1\}=S-\tfrac{1}{2}c'. \end{aligned} \tag{24}$$

The quantities c and c' have been calculated for cubic lattices by Anderson and Kubo.[7] These results are in agreement with Oguchi.

At finite but low temperatures we may find an iterative solution for the small quantity $\alpha-\alpha_0$. This gives

$$\alpha=\alpha_0-\frac{3\zeta(4)}{\pi^2\eta^3S(1+\alpha_0)^4}\left(\frac{kT}{h_e}\right)^4-\frac{36[\zeta(4)]^2}{\pi^4\eta^6S^2(1+\alpha_0)^9}\left(\frac{kT}{h_e}\right)^8. \tag{25}$$

[7] P. W. Anderson, Phys. Rev. **86**, 694 (1952); R. Kubo, *ibid.* **87**, 568 (1952).

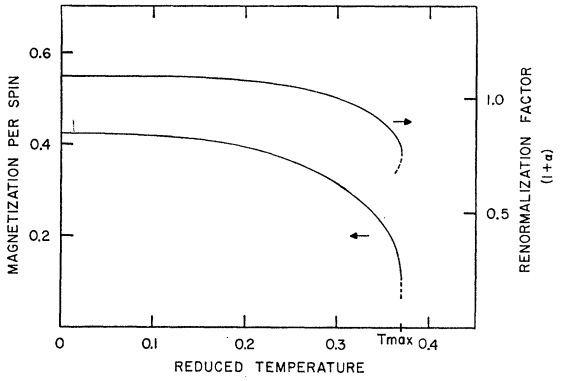

FIG. 1. The renormalization factor and the sublattice magnetization of a simple cubic antiferromagnet as calculated from the theory.

From this we find the energy and the magnetization

$$\begin{aligned} E&=E_0+\frac{3Nh_e\zeta(4)}{\pi^2\eta^3(1+\alpha_0)^3}\left(\frac{kT}{h_e}\right)^4 \\ &\quad+\left(\frac{63}{2}\right)\frac{N[\zeta(4)]^2}{\pi^4\eta^6S(1+\alpha_0)^8}\left(\frac{kT}{h_e}\right)^8, \\ m&=m_0-\frac{\zeta(2)}{2\pi^2\eta^3(1+\alpha_0)^2}\left(\frac{kT}{h_e}\right)^2 \\ &\quad-\frac{3\zeta(2)\zeta(4)}{\pi^4\eta^6S(1+\alpha_0)^7}\left(\frac{kT}{h_e}\right)^6, \end{aligned} \tag{26}$$

where the quantity η has been defined and tabulated by Oguchi. The last term of each expression arises from the spin-wave interaction. The terms arising from the nonparabolic shape of the dispersion curve have been left out. These reduce to the Oguchi results if we ignore α_0 in the spin-wave interaction terms.

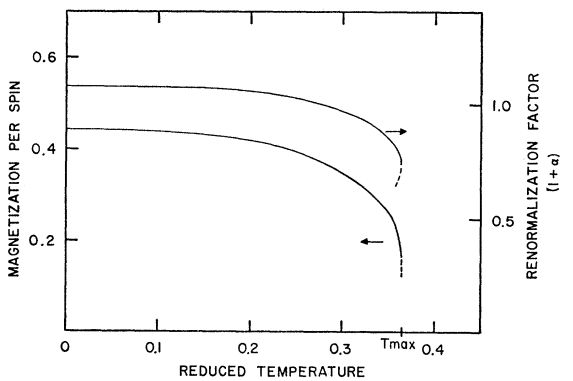

FIG. 2. The renormalization factor and the sublattice magnetization of a body-centered cubic antiferromagnet as calculated from the theory.

TABLE I. Comparison of T_{max} with estimations of T_N.

Lattice	kT_N/J BPW approx.	kT_N/J Tyablikov approx.	kT_{max}/J Present theory
Simple cubic	2.00	1.98	2.21
Body-centered cubic	3.18	2.87	2.91
One-dimensional	None	None	0.84

IV. HIGH-TEMPERATURE RESULTS

At high temperatures the equation for α has been solved numerically and the dependence of the quantity $(1+\alpha)$ on the temperature is plotted for simple cubic (sc) and body-centered cubic lattices in Figs. 1 and 2. On the same graphs we also plot the sublattice magnetization per spin. It can be seen that, just as in the ferromagnetic case, the magnetization drops with increasing temperature faster than the renormalization factor $(1+\alpha)$. Also, the equation for α has no solution above a certain temperature T_{max}, whose value is found to be (for $S=\frac{1}{2}$)

$$kT_{max}/h_e=0.369\pm0.001 \quad \text{for sc},$$
$$=0.364\pm0.001 \quad \text{for bcc}.$$

It is interesting to note that these values are very close to the other theoretical estimates for the Néel temperature. A comparison is given in Table I where the first column lists the estimations of Li[8] based on the Bethe-Peierls-Weiss (BPW) approximation and the second column the values based on the Tyabilikov approximation. The latter theory as was first proposed by Pu[9] and later elaborated by Lines.[10]

Since the present theory ignores the kinematic interaction between the spin waves, the nature of the instability at T_{max} is quite different from the phase transition at the Néel temperature. However, as can be seen from the figures, the magnetization decreases rapidly toward zero near T_{max}, which is just the expected behavior of a real system near T_N. This may be the reason why the two temperatures are so close. In a one-dimensional system it is easy to verify that the sublattice magnetization diverges. Also, most existing theories predict that the system has no phase transition. The present theory, however, gives $kT_{max}/J=0.84$ for $S=\frac{1}{2}$. Therefore, when the magnetization does not exist, T_{max} also loses its meaning. It seems likely that the instability at T_{max} has no physical significance but is rather a consequence of the approximation.

V. SUSCEPTIBILITIES

Using the Kubo method for linear response function,[11] we can write the parallel susceptibility of the system in terms of spin-correlation functions as

$$\chi_{\parallel}=(g\mu_B)N^2\int_0^\beta \langle TS_0^z(\tau)S_0^z(0)\rangle d\tau, \tag{27}$$

where

$$S_0^z=N^{-1}[\textstyle\sum_i S_{1i}^z+\sum_j S_{2j}^z]$$
$$=N^{-1}\textstyle\sum_k [c_k^*c_k-d_k^*d_k], \tag{28}$$

after a transformation to the spin-wave variables. It can be easily verified that S_0^z commutes with the Hamiltonian, so

$$\chi_{\parallel}=g\mu_B\beta\textstyle\sum_{kk'}\langle(c_k^*c_k-d_k^*d_k)(c_{k'}^*c_{k'}-d_{k'}^*d_{k'})\rangle.$$

After taking the thermal average, all terms with $\mathbf{k}\neq\mathbf{k}'$ cancel out in the sum. The terms with $\mathbf{k}=\mathbf{k}'$ can be calculated by transforming to the quasiparticle operators and using the standard method. The result is

$$\chi_{\parallel}=2g\mu_B\beta\textstyle\sum_k e^{\beta\omega_k}[e^{\beta\omega_k}-1]^{-2}. \tag{29}$$

In a similar manner, the perpendicular susceptibility has the expression

$$\chi_{\perp}=g\mu_BN^2\int_0^\beta \langle TS_0^x(\tau)S_0^x(0)\rangle d\tau$$
$$=g\mu_BN^2\beta\langle S_0^xS_0^x\rangle, \tag{30}$$

where

$$S_0^x=N^{-1}[\textstyle\sum_i S_{1i}^x+\sum_j S_{2j}^x],$$

and

$$S_{1i}^x=\tfrac{1}{2}(S_{1i}^+ +S_{1i}^-)$$
$$=(S/2)^{1/2}[b_{1i}+b_{1i}^*-(2S)^{-1}b_{1i}^*b_{1i}b_{1i}], \tag{31}$$
$$S_{2j}^x=(S/2)^{1/2}[b_{2j}^*+b_{2j}-(2S)^{-1}b_{2j}^*b_{2j}^*b_{2j}].$$

The thermal average is easy to evaluate and the result is

$$\chi_{\perp}=\tfrac{1}{2}(g\mu_BN)S\beta[1-2(NS)^{-1}\textstyle\sum_k n_k](2n_0+2\xi_0+1). \tag{32}$$

The factor

$$S[1-2(NS)^{-1}\textstyle\sum_k n_k]=m$$

is just the sublattice magnetization per spin. The quantities n_0 and ξ_0 both diverge but the sum $2n_k+2\xi_k+1$

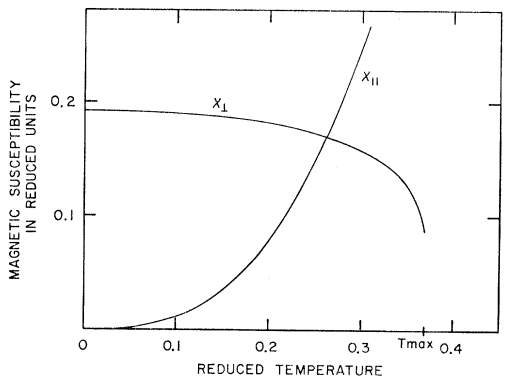

FIG. 3. The theoretical temperature dependence of $\chi_{\parallel}$ and $\chi_{\perp}$ for a simple cubic antiferromagnet.

[8] Y. Y. Li, Phys. Rev. 84, 721 (1951).
[9] F. -C. Pu, Dokl. Akad. Nauk SSSR 130, 1244 (1960) [English transl.: Soviet Phys.—Doklady 5, 128 (1960)].
[10] M. E. Lines, Phys. Rev. 135, A1336 (1964).
[11] R. Kubo, J. Phys. Soc. Japan 12, 570 (1957).

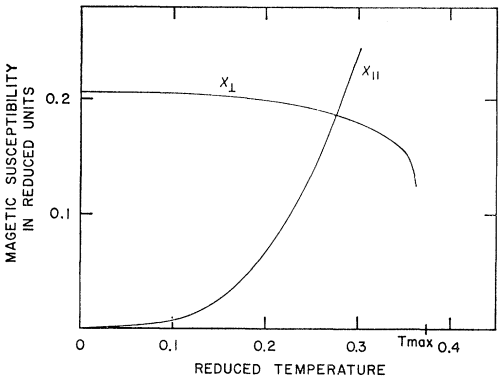

FIG. 4. The theoretical temperature dependence of $\chi_{||}$ and $\chi_\perp$ for a body-centered cubic antiferromagnet.

has a finite limit as $k \to 0$. This limit is found to be

$$2n_0+2\xi_0+1=[\beta h_e(1+\alpha)]^{-1}.$$

Thus,

$$\chi_\perp = m(g\mu_B N)/2h_e(1+\alpha). \tag{33}$$

At low temperatures both Eqs. (29) and (34) reduce to the Oguchi results. Figures (3) and (4) show the behavior of the susceptibilities at high temperatures. The initial T^2 dependence of $\chi_{||}$ and the initial drop of $\chi_\perp$ are as predicted by the Oguchi theory. However, it appears that $\chi_\perp$ drops too drastically and $\chi_{||}$ rises too sharply near $T_{\max}$. This seems to indicate also that the theory does not apply in this temperature region and the instability at $T_{\max}$ is unrelated to the phase transition at the Néel temperature.

VI. DISCUSSION

There is one simple antiferromagnetic model that permits some rigorous analysis, i.e., the one-dimensional model for spin $\frac{1}{2}$. This serves as a gauge to measure the success of any theory of antiferromagnetism. For the Hamiltonian in Eq. (1), the exact ground-state energy is[12]

$$E_0(\text{exact}) = -(2\ln 2-\tfrac{1}{2})NJ = -0.8863NJ,$$

and the excitation spectrum at 0°K is[13]

$$\omega_k(\text{exact}) = (\pi/2)|\sin k| = 1.57|\sin k|.$$

From the present calculation we find at 0°K that

$$\alpha = 1-(2\pi)^{-1}\int_{-\pi}^{\pi}|\sin k|\,dk$$
$$= 1-2/\pi.$$

This gives the approximate ground-state energy and excitation spectrum

$$E_0 = -\tfrac{1}{2}NJ(2-2/\pi)^2 = -0.926NJ,$$
$$\omega_k = (2-2/\pi)|\sin k| = 1.36|\sin k|,$$

whereas the Anderson theory gives

$$E_0 = -(\tfrac{3}{2}-2/\pi)NJ = -0.863NJ,$$
$$\omega_k = |\sin k|.$$

It is seen by comparing these results that the present theory gives a better spin-wave spectrum at 0°K but the ground-state energy is too low. Together with the simple spin-wave theory we get the upper and lower bounds of the ground-state energy.

We may further speculate that the above conclusion perhaps applies to three-dimensional systems as well. If so, then the ground-state energy should satisfy

$$-\tfrac{1}{2}Nh_e(S+c) > E_0 > -\tfrac{1}{2}Nh_e(S+c+c^2/4S).$$

Since $c^2/4S$ is a 1% correction, we may conclude that the simple spin-wave theory should give a very accurate value for the ground-state energy of three-dimensional antiferromagnets.

Korringa[14] suggested a different correction factor for the spin-wave spectrum in the long-wavelength limit. Following the argument of Keffer and Loudon,[15] he postulated that the correction factor to the spin-wave energy should be the same as that for the ground-state energy in the simple spin-wave theory. The latter factor is easily found to be $(1+2\alpha)$ and so he obtains

$$\omega_k = (1+2\alpha)[1-\gamma^2(\mathbf{k})]^{1/2}. \tag{34}$$

For a one-dimensional system, this works out to be

$$\omega_k = 1.72|\sin k|,$$

which is rather close to the exact result. Unfortunately, his theory, which gives support to Eq. (34), does not seem to apply to one-dimensional systems.

ACKNOWLEDGMENTS

The author is grateful to Dr. D. C. Mattis for helpful discussions and kind encouragements. He is also indebted to Dr. S. H. Charap for an illuminating discussion on the Maleev transformation.

[12] L. Hulthén, Arkiv Mat. Astron. Fysik **26A**, No. 11 (1938).
[13] J. des Cloizeaux and J. J. Pearson, Phys. Rev. **128**, 2131 (1962).
[14] J. Korringa, Phys. Rev. **125**, 1972 (1962).
[15] F. Keffer and R. Loudon, Suppl. J. Appl. Phys. **32**, 2 (1961).