Unification of Extant Theories of the Heisenberg Ferromagnet

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Four recently proposed theories of the Heisenberg ferromagnet have been examined within a Green function formulation. The decoupling parameters were chosen for each theory so that the expressions for the renormalization factor and the magnetization are identical to those originally derived. Comparisons of the approximations introduced and of the results are more readily made within this single theoretical framework. The temperature dependence of the magnetization has been numerically computed for each of the four theories for simple cubic, body-centered cubic, and face-centered cubic lattices with spin $\frac{1}{2}$.

I. INTRODUCTION

THE statistical mechanics of a Heisenberg model of a ferromagnet have been studied rigorously in both the low-temperature[1–4] and high-temperature[5–8] regions. Although rigorous solutions have not been found for the intermediate region, numerous approximate theories[9–21] have been developed which include this temperature range. Since various techniques have been used to develop these theories, it is often difficult to compare the approximations used in the development and thereby understand the physical basis for similarities or differences in the theoretical predictions.

We consider four recently proposed theories (M. Bloch,[15] random phase approximation[16] or Tyablikov,[18] Oguchi-Honma,[20] and Callen[21]) which have had varying degrees of success when compared with the rigorous low- and high-temperature results.

The M. Bloch[15] theory was developed by retaining in the Hamiltonian the diagonal terms up to fourth order in the Holstein-Primakoff[22] creation and annihilation operators and assuming that this truncated Hamiltonian remains valid through the entire temperature range. The resulting expression for the magnetization agrees with the Dyson[1] expansion at low temperatures (i.e., the leading correction due to magnon interactions is of the order of T^4); as the temperature is increased, it is found that no self-consistent solution exists above a certain maximum temperature. This maximum temperature agrees favorably with Curie temperatures obtained from the rigorous high-temperature expansions; however, the magnetization is not zero at this maximum temperature, but has a value of about $\frac{1}{3}$ of the saturation value.

The random phase approximation of Englert[16] (the results of which are identical to those given by Tyablikov[18] in terms of double time-temperature-dependent Green functions) consists of approximating the commutation relations of the Fourier components of spin operators to the extent of replacing the commutation relation $[S_{k+\lambda}{}^+,S_\lambda{}^-]=2S_k{}^z$ by $[S_{k+\lambda}{}^+,S_\lambda{}^-]=2\langle S^z\rangle\delta_{k,0}$. The low-temperature expansion of the resulting expression for the magnetization contains a T^3 term and, therefore, does not agree with Dyson.[1] The magnetization exhibits a definite Curie temperature at which the spontaneous magnetization vanishes; this Curie temperature compares favorably with the rigorous results.

The Oguchi-Honma[20] and Callen[21] theories were both developed using the techniques of double time-temperature-dependent Green functions. However, Oguchi and Honma[20] express the spin operators in terms of the Holstein-Primakoff[22] boson operators through the use of the Oguchi transformation,[23] while Callen[21] treats the spin operators directly. Both theories introduce decoupling approximations in order to solve the Green function equation of motion, and both theories give terms in the low-temperature expansion of the magnetization in addition to those found rigorously. (The leading additional term is a $T^{3S+3/2}$ term, which for spin $\frac{1}{2}$ is T^3.) Since the theories have identical low-temperature behavior, it is plausible that in this limit the approximations made are identical. However, at higher temperatures the theories differ markedly. The Oguchi-Honma

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theory predicts an infinite Curie temperature[24]; the magnetization asymptotically approaches zero as the temperature approaches infinity. In contrast, the Callen theory predicts a definite finite Curie temperature at which the spontaneous magnetization vanishes. While this Curie temperature is somewhat high compared to the rigorous results for spin $\frac{1}{2}$, the Callen Curie temperatures show good agreement as the magnitude of the spin becomes larger (as Callen[21] has shown, the Curie temperature is quite sensitive to the decoupling approximation, and the Callen Curie temperatures can easily be made identical to those of Tyablikov[18] and Tahir-Kheli and ter Haar[19] without altering the low- and high-temperature behavior of the Callen theory).

We formulate these four theories for the case of nearest-neighbor exchange interactions and spin $\frac{1}{2}$ in a Green function calculation using an extended decoupling approximation involving two decoupling parameters. The choice of one of the decoupling parameters determines the form of the expression for the transverse correlation function and, therefore, the magnetization. Thus, this parameter is uniquely determined for each theory by demanding that the expression for the magnetization be identical to that obtained from each of the theories as originally derived. The quasiparticle energies as given by all four theories are equivalent to simple spin-wave energies "renormalized" by a factor which is dependent upon the number of excitations and, therefore, upon the temperature. The renormalization factors obtained by these theories all differ. Since the form of this factor is dependent upon the choice of both decoupling factors, and since the choice of one of these parameters is dictated by the form of the expression for the magnetization, the other decoupling parameter can be determined for each theory by demanding that the renormalization factor in each case be identical to that obtained in the original derivation. We are then able to discuss the similarities and differences of the theories in terms of the similarities and differences of the decoupling parameters and their physical implications.

As an aid in making these comparisons, we have numerically computed the temperature dependence of the magnetization for each of the four theories for simple cubic, body-centered cubic, and face-centered cubic lattices with spin $\frac{1}{2}$. These calculations show that the temperature dependence of the magnetization of the four theories is very nearly identical in the low-temperature region despite the difference in the low-temperature expansions of the magnetization; the higher temperature behavior shows marked differences. The curves of the magnetization versus the normalized temperature (T divided by T_{Curie}) show little structural dependence for any of the four theories. For the random phase and Callen theories, the magnetization is found to vary as $(1-T/T_C)^{1/2}$, in the temperature range $T_C/2$ to T_C. The calculations also confirm[24] the infinite Curie point of the Oguchi-Honma theory.

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II. GREEN FUNCTION FORMULATION

We consider the Hamiltonian

$$\mathcal{H}=-\mu H_0\sum_g S_g{}^z-J\sum_{g,\delta}\mathbf{S}_g\cdot\mathbf{S}_{g+\delta}\,, \tag{1}$$

where μS is the magnetic moment per ion; H_0 is the applied magnetic field, which we assume to be in the negative z direction; $\mathbf{S}_g$ is the spin operator (in units of $\hbar$) for the ion at site g; $\boldsymbol{\delta}$ is a vector connecting the gth site with a nearest neighbor. We restrict our attention to simple lattices (including, in particular, simple cubic, body-centered cubic, and face-centered cubic lattices) with spin $\frac{1}{2}$ and nearest-neighbor exchange interactions; J is the nearest-neighbor exchange integral.

The temperature-dependent retarded Green function[25] involving the operators $S_g{}^+(t)$ and $S_l{}^-$ is defined by

$$\langle\langle S_g{}^+(t)\,;S_l{}^-\rangle\rangle\equiv-i\theta(t)\langle[S_g{}^+(t),S_l{}^-]\rangle\,, \tag{2}$$

where $\theta(t)$ is the step function which is unity for positive t and zero for negative t, $S^{\pm}=S^x\pm iS^y$, single square brackets denote a commutator, and single angular brackets denote an average with respect to the canonical density matrix of the system at temperature T. The Fourier transform (with respect to ω) of the Green function is denoted by

$$G_E(g,l)\equiv\langle\langle S_g{}^+(t)\,;S_l{}^-\rangle\rangle_E\,, \tag{3}$$

where $E=\hbar\omega$. The equation of motion which $G_E(g,l)$ satisfies is

$$EG_E(g,l)=\frac{1}{2\pi}\langle[S^+,S^-]\rangle\delta_{gl}+\langle\langle[S_g{}^+(t),\mathcal{H}]\,;S_l{}^-\rangle\rangle_E\,. \tag{4}$$

If Eq. (4) can be solved for $G_E(g,l)$, one can calculate the correlation function $\langle S_l{}^-S_g{}^+(t)\rangle$ from the relation

$$\langle S_l{}^-S_g{}^+(t)\rangle=\lim_{\epsilon\to0}i\int_{-\infty}^{\infty}\frac{G_{\hbar\omega+i\epsilon}(g,l)-G_{\hbar\omega-i\epsilon}(g,l)}{e^{(\hbar\omega/kT)}-1}e^{-i\omega t}d\omega\,. \tag{5}$$

As we shall see, the solution of Eqs. (4) and (5) enables us to obtain expressions for the dispersion relation and the magnetization.

The substitution into Eq. (4) of the expression obtained from the commutation of $S_g{}^+$ with the Hamiltonian yields

$$EG_E(g,l)=\frac{1}{2\pi}2\langle S^z\rangle\delta_{g,l}+\mu H_0G_E(g,l)+2J\sum_\delta\langle\langle(S_{g+\delta}{}^zS_g{}^+-S_g{}^zS_{g+\delta}{}^+)\,;S_l{}^-\rangle\rangle_E\,, \tag{6}$$

[25] See, for example, V. L. Bonch-Bruevich and S. V. Tyablikov, *Green-Function Methods in Statistical Mechanics* (translation) (North-Holland Publishing Company, Amsterdam, 1962).

where the commutator $[S^+,S^-]$ has been replaced by its value $2S^z$ and where δ indicates a sum over the nearest neighbors of the gth site. Equations of motion can be written for the higher order Green functions which appear on the right side of (6); these equations in turn involve still higher order Green functions. At some point these equations of motion must be decoupled in order to obtain an explicit solution for $G_E(g,l)$. Generally the procedure has been to make a decoupling approximation directly in Eq. (6). Tyablikov[18] has suggested that the Green functions of the form $\langle\langle S_g{}^zS_f{}^+;S_l{}^-\rangle\rangle_E$ should be approximated by ignoring the fluctuations in $S_g{}^z$, that is, by replacing $S_g{}^z$ by its average value, and

$$\langle\langle S_g{}^zS_f{}^+;S_l{}^-\rangle\rangle_E \underset{g\neq f}{\rightarrow} \langle S^z\rangle\langle\langle S_f{}^+;S_l{}^-\rangle\rangle. \quad (7)$$

Callen[21] has suggested an alternative method for decoupling which attempts to account for the correlation of S^z on one site with the transverse spin on another. He proposed that the Green function

$$\langle\langle S_g{}^-S_g{}^+S_f{}^+;S_l{}^-\rangle\rangle_E$$

be decoupled in the symmetric form

$$\langle\langle S_g{}^-S_g{}^+S_f{}^+;S_l{}^-\rangle\rangle_E \underset{g\neq f}{\rightarrow} \langle S_g{}^-S_g{}^+\rangle\langle\langle S_f{}^+;S_l{}^-\rangle\rangle_E$$
$$+\langle S_g{}^-S_f{}^+\rangle\langle\langle S_g{}^+;S_l{}^-\rangle\rangle_E+\langle S_g{}^+S_f{}^+\rangle\langle\langle S_g{}^-;S_l{}^-\rangle\rangle_E. \quad (8)$$

The last term on the right side of Eq. (8) vanishes for the Hamiltonian we are considering since $S_g{}^+S_f{}^+$ is not diagonal in $S_{\text{total}}{}^z$, but, in general, it must be included (for example, if the dipolar interaction is included in the Hamiltonian).[26]

For spin $\frac{1}{2}$ (the procedure has been generalized by Callen for arbitrary spin), $S_g{}^z$ can be written as

$$S_g{}^z=S-S_g{}^-S_g{}^+ \quad (9)$$

or

$$S_g{}^z=\tfrac{1}{2}(S_g{}^+S_g{}^--S_g{}^-S_g{}^+). \quad (10)$$

Multiplying Eq. (9) by α and Eq. (10) by $1-\alpha$ and adding the resultant equations yields

$$S_g{}^z=\alpha S+\frac{1-\alpha}{2}S_g{}^+S_g{}^--\frac{1+\alpha}{2}S_g{}^-S_g{}^+. \quad (11)$$

Equations (8) and (11) lead to

$$\langle\langle S_g{}^zS_f{}^+;S_l{}^-\rangle\rangle_E \underset{g\neq f}{\rightarrow} \langle S^z\rangle\langle\langle S_f{}^+;S_l{}^-\rangle\rangle_E$$
$$-\alpha\langle S_g{}^-S_f{}^+\rangle\langle\langle S_g{}^+;S_l{}^-\rangle\rangle_E. \quad (12)$$

The operator $S_g{}^-S_g{}^+$ in Eq. (9) represents the deviation of $\langle S^z\rangle$ from S. It is this operator which is treated approximately when decoupling on the basis of Eq. (9), i.e., choosing $\alpha=1$. Therefore, Callen proposes Eq. (9) ($\alpha=1$) as the basis for decoupling when the deviation of $\langle S^z\rangle$ from S is small, i.e., in the low-temperature region.

Similarly, the operator $\frac{1}{2}(S_g{}^+S_g{}^--S_g{}^-S_g{}^+)$ in Eq. (10) represents the deviation of $\langle S^z\rangle$ from 0, and Callen proposes that Eq. (10) ($\alpha=0$) be used as the basis for decoupling as $\langle S^z\rangle$ approaches 0. The argument for the use of Eq. (10) is not as transparent as that for the use of Eq. (9), for although the difference in the operators S^+S^- and S^-S^+ is small if $\langle S^z\rangle\cong 0$, each operator makes a contribution of the order of S, and it is each operator which is treated approximately, not the difference. Nevertheless, as we shall see, the $\alpha=0$ decoupling approximation seems to be appropriate in the $\langle S^z\rangle\cong 0$ limit. On the basis of the above observations, Callen chooses (for spin $\frac{1}{2}$)

$$\alpha=2\langle S^z\rangle \quad (13)$$

so that $\alpha\rightarrow 1$ as $\langle S^z\rangle\rightarrow\frac{1}{2}$ and $\alpha\rightarrow 0$ as $\langle S^z\rangle\rightarrow 0$. [The choice of $\alpha=0$ over the entire temperature range is just Tyablikov decoupling since Eq. (12) becomes identical to Eq. (7).] We shall carry α explicitly throughout the calculation and let it be determined for each theory by fitting the results to those obtained in the original derivation as indicated in the Introduction.

Finally, Wortis[27] has indicated that the higher order Green function is equal to a proportionality factor times the lower order Green function plus an additional term. Tahir-Kheli[28] has determined the form of both the proportionality factor (the "mass operator") and the additional term by requiring agreement of the resulting theory with rigorous results obtained from the low- and high-temperature expansions. We shall introduce this additional term as a second decoupling parameter to be determined for each of the four theories. Thus, we use a decoupling approximation

$$\langle\langle S_g{}^zS_f{}^+;S_l{}^-\rangle\rangle_E \underset{g\neq f}{\rightarrow} \langle S^z\rangle\langle\langle S_f{}^+;S_l{}^-\rangle\rangle_E$$
$$-\alpha\langle S_g{}^-S_f{}^+\rangle\langle\langle S_g{}^+;S_l{}^-\rangle\rangle_E+\rho(g,f,l), \quad (14)$$

where $\rho(g,f,l)$ is a function of the relative positions of the g, f, and l sites. Insertion of the decoupling approximation [Eq. (14)] into the equation of motion [Eq. (6)] yields

$$EG_E(g,l)=\frac{1}{2\pi}2\langle S^z\rangle\delta_{g,l}+\mu H_0G_E(g,l)$$
$$+2J\langle S^z\rangle\sum_\delta[G_E(g,l)-G_E(g+\delta,l)]$$
$$+2J\alpha\sum_\delta[\langle S_g{}^-S_{g+\delta}{}^+\rangle G_E(g,l)$$
$$-\langle S_{g+\delta}{}^-S_g{}^+\rangle G_E(g+\delta,l)]$$
$$+2J\sum_\delta[\rho(g+\delta,g,l)-\rho(g,g+\delta,l)]. \quad (15)$$

[26] C. W. Haas, Phys. Rev. **132**, 228 (1963).

[27] M. Wortis, Ph.D. dissertation, Harvard University, 1963 (unpublished).

[28] R. A. Tahir-Kheli, Phys. Rev. **132**, 689 (1963).

Since the last term on the right side of Eq. (15) depends only on the positions of the g and l sites, we shall denote that term as $\beta(g,l)/2\pi$. We introduce the Fourier transforms dictated by translational invariance

$$G_E(k)=\sum_{\mathbf{g}-\mathbf{l}} e^{-i(\mathbf{g}-\mathbf{l})\cdot\mathbf{k}}G_E(g,l)\,, \tag{16}$$

$$\psi(k)=\sum_{\mathbf{g}-\mathbf{l}} e^{-i(\mathbf{g}-\mathbf{l})\cdot\mathbf{k}}\langle S_l^-S_g^+\rangle\,, \tag{17}$$

$$\gamma_k=\frac{1}{z}\sum_{\delta} e^{i\mathbf{k}\cdot\delta}\,, \tag{18}$$

$$\beta_k=\sum_{\mathbf{g}-\mathbf{l}} \beta(g,l)e^{-i(\mathbf{g}-\mathbf{l})\cdot\mathbf{k}}\,, \tag{19}$$

where z is the number of nearest neighbors and $(\mathbf{g}-\mathbf{l})\cdot\mathbf{k}$ denotes the vector products $\mathbf{r}_{gl}\cdot\mathbf{k}$. From (15), (16), (17), (18), and (19), we find

$$G_E(k)=\frac{(2\langle S^z\rangle+\beta_k)}{2\pi(E-E_k)}\,, \tag{20}$$

where

$$E_k=\mu H_0+2Jz\langle S^z\rangle(1-\gamma_k)+\frac{2Jz\alpha}{N}\sum_{k'}(\gamma_{k'}-\gamma_{k'-k})\psi_{k'}\,. \tag{21}$$

It has been shown[15,21] that for lattices exhibiting cubic symmetry, Eq. (21) can be rewritten in the form

$$E_k=\mu H_0+Jz(1-\gamma_k)\left(2\langle S^z\rangle+\frac{2\alpha}{N}\sum_{k'}\gamma_{k'}\psi_{k'}\right). \tag{22}$$

The Fourier transform of the correlation function $\langle S_l^-S_g^+\rangle$ can be obtained from the Green function (20) by the use of Eq. (5) and is easily shown to be

$$\psi_k=(2\langle S^z\rangle+\beta_k)\varphi_k\,, \tag{23}$$

where

$$\varphi_k=1/(e^{E_k/kT}-1)\,. \tag{24}$$

Thus,

$$E_k=\mu H_0+\epsilon_k R\,, \tag{25}$$

where

$$\epsilon_k=Jz(1-\gamma_k)\,, \tag{26}$$

the energy of a spin wave of wave vector $\mathbf{k}$ in the absence of an external magnetic field, and R is the renormalization factor given by the expression

$$R=2\langle S^z\rangle+\frac{2\alpha}{N}\sum_k(2\langle S^z\rangle+\beta_k)\gamma_k\varphi_k\,. \tag{27}$$

For these lattices and nearest-neighbor isotropic exchange interactions, the renormalization factor R is not a function of the wave vector. Since, for spin $\frac{1}{2}$,

$$\langle S^z\rangle=\tfrac{1}{2}-\langle S_g^-S_g^+\rangle\,, \tag{28}$$

from (23) we find that

$$\langle S^z\rangle=\tfrac{1}{2}-2\langle S^z\rangle\Phi+\frac{1}{N}\sum_k\beta_k\varphi_k\,, \tag{29}$$

where

$$\Phi=\frac{1}{N}\sum_k\varphi_k\,. \tag{30}$$

For our discussion, we shall assume $\beta(g,l)$ to have the form $\beta\delta_{g,l}$, i.e., the additional decoupling parameter affects only the Green function $G_E(g,g)$.[29] For this case, (27) and (29) simplify to

$$R=2\langle S^z\rangle+\frac{2\alpha(2\langle S^z\rangle+\beta)}{N}\sum_k\gamma_k\varphi_k\,, \tag{31}$$

and

$$\langle S^z\rangle=\tfrac{1}{2}-(2\langle S^z\rangle+\beta)\Phi\,, \tag{32}$$

or, alternatively,

$$\langle S^z\rangle=(\tfrac{1}{2}-\beta\Phi)/(1+2\Phi)\,. \tag{33}$$

III. DECOUPLING PARAMETERS

The decoupling parameters α and β are chosen for each theory by first demanding that the expression (32) for $\langle S^z\rangle$ be identical to that originally obtained for each theory. This value of β is then inserted into Eq. (31) for R and α chosen for each theory by demanding that expression (31) then be identical to the renormalization factor originally obtained for each theory.

The expressions for $\langle S^z\rangle$ and R as given by each of the four theories are listed in Table I. The Bloch expression[15] for the average value of S^z

$$\langle S^z\rangle=\tfrac{1}{2}-\Phi \tag{34}$$

is identical in form to that obtained by spin-wave theory and has been assumed by Bloch to be valid over the entire temperature range if ϵ_k is replaced by E_k. This expression can be obtained from (32) if

$$\beta=1-2\langle S^z\rangle \tag{35}$$

which is equivalent to assuming

$$\beta=2\Phi\,. \tag{36}$$

This choice of β is therefore equivalent to assuming that each excited quasiparticle decreases M_z, the z component of the magnetization, by an amount $\gamma\hbar$. The expressions for $\langle S^z\rangle$ for the other three theories[19–21] are identical.

$$\langle S^z\rangle=\tfrac{1}{2}/(1+2\Phi)\,. \tag{37}$$

This result is obtained from (33) by setting $\beta=0$, which is, of course, the decoupling approximation which has been made in these cases. This choice of β is equivalent to assuming that each excited quasiparticle decreases M_z by an amount $2\gamma\hbar\langle S^z\rangle$, i.e., the effect of additional excitations on M_z decreases. The values of α necessary

[29] A. C. Hewson and D. ter Haar, Physics Letters **6**, 136 (1963).

TABLE I. Renormalization factor, expression for $\langle S^z\rangle$, and decoupling parameters for each of the four theories.

Theory	R	$\langle S^z\rangle$	α	β
Bloch	$2\langle S^z\rangle+\frac{2}{N}\sum_k \gamma_k\varphi_k$	$\frac{1}{2}-\Phi$	1	2Φ (i.e., $1-2\langle S^z\rangle$)
Oguchi-Honma	$2\langle S^z\rangle+\frac{4\langle S^z\rangle}{N}\sum_k \gamma_k\varphi_k$	$\frac{\frac{1}{2}}{1+2\Phi}$	1	0
Callen	$2\langle S^z\rangle+\frac{8\langle S^z\rangle^2}{N}\sum_k \gamma_k\varphi_k$	$\frac{\frac{1}{2}}{1+2\Phi}$	$2\langle S^z\rangle$	0
Random phase approximation	$2\langle S^z\rangle$	$\frac{\frac{1}{2}}{1+2\Phi}$	0	0

to give the appropriate renormalization factors are now easily determined from (31). The values of α and β for each of the theories are listed in Table I.

We consider first the low-temperature region with zero external field ($H_0=0$). By the standard low-temperature series expansions,[1] it can be easily shown that for all four theories

$$\Phi=\zeta(\tfrac{3}{2})\tau^{3/2}+\tfrac{3}{4}\pi\nu\zeta(\tfrac{5}{2})\tau^{5/2}+\pi^2\omega\nu^2\zeta(\tfrac{7}{2})\tau^{7/2}+\cdots$$
$$+3(1-\alpha)\zeta^2(\tfrac{3}{2})\tau^3+3\pi\nu\zeta(\tfrac{3}{2})\zeta(\tfrac{5}{2})\tau^4(2-\alpha)+\cdots, \quad (38)$$

where we have retained terms up to τ^4 in the expansion and where $\zeta(x)$ is the Riemann zeta function,

$$\tau\equiv 3kT/2\pi zJ\gamma \quad (39)$$

and the structure-dependent constants are

simple cubic	$\nu=1$,	$\omega=33/32$	
body-centered cubic	$\nu=\frac{3}{4}\times 2^{2/3}$,	$\omega=281/288$	(40)
face-centered cubic	$\nu=2^{1/3}$,	$\omega=15/16$.	

Substitution of (38) with $\alpha=1$ into (34) yields the Dyson result as calculated in the first Born approximation, and the Bloch theory is, therefore, successful in this limit.

In contrast, the substitution of (38) into (37) with any of the values of α shown in Table I does not give Dyson's result. In the low-temperature region where Φ is small, (37) becomes

$$\langle S^z\rangle\cong\tfrac{1}{2}-\Phi+2\Phi^2+\cdots. \quad (41)$$

Since Φ contains a $T^{3/2}$ term, the Φ^2 term makes a contribution to a T^3 term (plus other terms). This Φ^2 term is the source of the low-temperature difficulty in both the Oguchi-Honma and Callen theories. If the Φ^2 term were not present, these theories would also agree with the Dyson result (to order T^4) since both theories have values of α which in the low-temperature limit correspond to $\alpha=1$. For general spin, the analog of (41) is

$$\langle S^z\rangle\cong S-\Phi+(2S+1)\Phi^{2S+1}. \quad (42)$$

Thus, for larger spins, the additional terms given by the Oguchi-Honma and Callen theories are higher order in T (e.g., for $S=1$, $T^{9/2}$, etc.).

The random phase approximation corresponds to a decoupling with $\alpha=0$. From (38) we find that Φ contains a T^3 term. Substitution of this expression into (41) yields a T^3 contribution from both the Φ and the Φ^2 terms which partially cancel; however, there is a net T^3 contribution to $\langle S^z\rangle$.

Therefore, the only theory which agrees satisfactorily with the rigorous results at low temperatures is the Bloch theory. The requirement that α approach 1 in the low-temperature limit is not sufficient; in addition, it is necessary that $\beta=2\Phi$ (that is, that $2\langle S^z\rangle+\beta$ be unity to a certain order in T; this order in T determines the lowest order spurious term in $\langle S^z\rangle$) in this temperature region in order to eliminate the spurious terms which otherwise appear in the low-temperature expansion.

We now consider the Curie temperatures predicted by each theory. We are therefore interested in the case of $H_0=0$ and $\langle S^z\rangle\rightarrow 0$. We first consider the random phase approximation, the Callen and the Oguchi-Honma theories for which the magnetization ($\beta=0$) can be expressed as

$$\langle S^z\rangle=\tfrac{1}{2}/(1+2\Phi). \quad (43)$$

For these theories, as $\langle S^z\rangle\rightarrow 0$, the quasiparticle spectrum collapses and Φ, the mean number of excited quasiparticles, tends to infinity as required by (43). In the limit of $\langle S^z\rangle$ small and Φ large

$$\langle S^z\rangle\Phi \xrightarrow[\langle S^z\rangle\rightarrow 0]{} \tfrac{1}{4}. \quad (44)$$

Since $\langle S^z\rangle\rightarrow 0$, we expand the Bose factors in Φ using (24), (25), (30), and (31) and find that the Curie temperature is given by the expression

$$\frac{kT_c}{Jz}=\left[1+\frac{2\alpha}{N}\sum_k \gamma_k\varphi_k\right]\Big/2F(-1), \quad (45)$$

where

$$F(-1)=\frac{1}{N}\sum_k \frac{1}{1-\gamma_k} \tag{46}$$

has been evaluated for the cubic lattices,[30] and where it is implied that the quantity

$$\frac{2\alpha}{N}\sum_k \gamma_k\varphi_k \tag{47}$$

be evaluated in the limit of $\langle S^z\rangle \to 0$.

For the case of $\alpha=0$, Eq. (45) assumes the familiar form given by the random phase approximation

$$kT_c/Jz=1/2F(-1). \tag{48}$$

For the case of Callen decoupling, $\alpha=2\langle S^z\rangle$, the limiting value of

$$\frac{4\langle S^z\rangle}{N}\sum_k \gamma_k\varphi_k \tag{49}$$

can be obtained by again expanding the Bose factor, and Callen[21] has shown that in this case

$$kT_c/Jz=[F(-1)-\tfrac{1}{2}]/F^2(-1). \tag{50}$$

As Callen has noted, the Curie temperature is quite sensitive to the choice of α. If he had chosen $\alpha=(2\langle S^z\rangle)^{1+\epsilon}$, where ϵ is any positive constant, no matter how small, he would have obtained the random phase approximation Curie temperature since the limiting value of

$$(2\langle S^z\rangle)^{\epsilon}\times\left(\frac{4\langle S^z\rangle}{N}\sum_k \gamma_k\varphi_k\right) \tag{51}$$

is zero. The term in the bracket tends to a limit but $(2\langle S^z\rangle)^{\epsilon}$ tends to zero, and therefore the product tends to zero. (Such a choice of α, with ϵ vanishingly small, would have no effect on the low- or high-temperature behavior of the theory.)[30a] Similarly for ϵ negative, the limiting value of

$$\frac{1}{(2\langle S^z\rangle)^{|\epsilon|}}\frac{4\langle S^z\rangle}{N}\sum_k \gamma_k\varphi_k \tag{52}$$

is infinity. Therefore, in the Oguchi-Honma theory, where $\alpha=1$ ($\epsilon=-1$), the limiting value of

$$\frac{2}{N}\sum_k \gamma_k\varphi_k$$

is infinity. From (45) we see that the Oguchi-Honma theory predicts an infinite Curie temperature as first pointed out by Tahir-Kheli and Callen.[24]

For the M. Bloch theory, the expression for $\langle S^z\rangle$ is

$$\langle S^z\rangle=\tfrac{1}{2}-\Phi. \tag{53}$$

In this case, for $\langle S^z\rangle$ to vanish, Φ must be $\frac{1}{2}$. However, as we shall see more directly in the next section, the substitution of the Bloch renormalization factor into the expression for Φ results in an equation for $\langle S^z\rangle$ which over part of the temperature range has two positive solutions. There is a maximum temperature above which there is no self-consistent solution; however, the magnetization is not zero at this maximum temperature. The magnetization actually falls to zero at a somewhat lower temperature.

Therefore, in order to obtain a well-defined Curie point in the usual sense,[30a] it appears that in the limit of $\langle S^z\rangle \to 0$ it is necessary for $\beta\to 0$ and for $\alpha\to 0$ in such a way that

$$\frac{2\alpha}{N}\sum_k \gamma_k\varphi_k$$

is finite.

IV. MAGNETIZATION CURVES

In order to display the similarities and differences of the results of these theories, we have plotted the temperature dependence of the magnetization as predicted by each theory for simple cubic, body-centered cubic, and face-centered cubic lattices. These plots were obtained by finding numerically the self-consistent solution of the expressions for R and $\langle S^z\rangle$. The calculations were made using an IBM 1620. The sums over the Brillouin zone were performed using Gauss' approximate quadrature method. A measure of the convergence of this method is the comparison of the computed value of the Watson sum[30] [Eq. (46)] with the exact value. For example, for the face-centered cubic, we calculate the sum to be 1.34448 while the exact value is 1.34466. The resultant error in the Curie temperatures of the random phase and Callen theories are of the order of 0.1%. Similar results are obtained for the body-

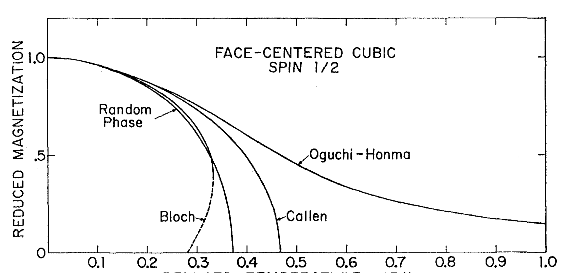

FIG. 1. A plot of the reduced magnetization $M(T)/M(0)$ versus the reduced temperature kT/Jz for each of the four theories for a face-centered cubic lattice and spin $\frac{1}{2}$. The form and relative positions of the curves for the body-centered and simple cubic lattices are very similar to those shown above.

[30] G. N. Watson, Quart. J. Math. **10**, 266 (1939); M. Tikson, J. Res. Natl. Bur. Std. **50**, 177 (1953).

[30a] *Note added in proof.* We have recently plotted the magnetization curves for various values of ϵ. For $0<\epsilon<\infty$, the magnetization does indeed vanish at a temperature corresponding to the random-phase approximation Curie temperature as given by Eq. (48). However, for these values of ϵ, the magnetization curves are double valued and bear a resemblance in form to the type of curve obtained from the Bloch theory as shown in Fig. 1.

centered cubic; however, the errors are somewhat larger for a simple cubic lattice. Caution must be used in relying upon the Watson sum alone as a criterion for convergence of the summing procedure. Even though the Watson sum converges rapidly as the number of points sampled increases, closely related sums may be found to converge much more slowly. The convergence of the Watson sum is an indication of the convergence of the summing procedure, but each sum must be reexamined on an individual basis.

In Fig. 1 we show the magnetization curves for the face-centered cubic lattice. Despite the differences in the low-temperature expansions, all four theories are very nearly identical in this region, i.e., $kT/12J<0.1$. The Oguchi-Honma curve was traced to higher temperatures than those shown in Fig. 1; for example, at a reduced temperature $(kT/12J)$ of 255, the magnetization is 3.7×10^{-4}.

The body-centered and simple cubic magnetization curves are very similar to those shown in Fig. 1 when plotted versus the appropriate reduced temperature kT/Jz. The curves can be brought into even closer agreement if the magnetizations are plotted versus the normalized temperature T/T_c, where T_c is the Curie temperature. Such curves are shown in Fig. 2 for the random phase, Callen and Bloch theories. The Bloch reduced temperature is normalized by using the maximum temperature for which there is a solution. The curves for the three lattices are represented by a single shaded line in Fig. 2: The upper edge of the line corresponds to the face-centered cubic curve; the lower edge to the simple cubic curve; the body-centered cubic curve lies close to that of the simple cubic. As can be seen from Fig. 2, the curves for each theory are very nearly independent of structure. (E. R. Callen[31] has made similar plots for the Callen theory for the face-centered cubic lattices with spin $\frac{1}{2}$ and spin $\frac{7}{2}$ and finds negligible spin dependence.) The Oguchi-Honma curves are in a sense already normalized since all have infinite Curie temperatures, and indeed the body-centered and simple cubic curves fall very nearly on the face-centered curve shown in Fig. 1; again the face-centered curve is slightly higher.

Tahir-Kheli and ter Haar[19,28] have found that just below the Curie temperature the magnetization of both

[31] E. R. Callen (private communication).

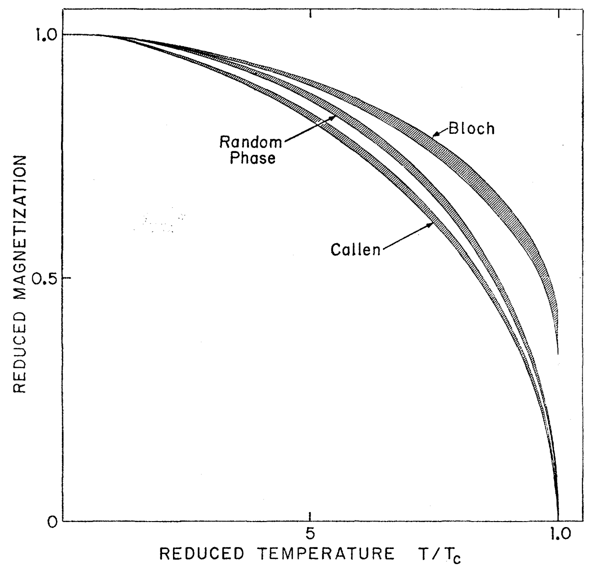

FIG. 2. A plot of the reduced magnetization $M(T)/M(0)$ versus the temperature normalized with respect to the Curie temperature T/T_c for each of the four theories. The band shown for each theory represents the spread in the magnetization curve due to structure. The upper edge of each band corresponds to the face-centered cubic lattice; the lower edge of each band corresponds to the simple cubic lattice. The body-centered cubic lattice curve lies in between but closer to that of the simple cubic.

the random phase and the Callen theories varies as $(1-T/T_c)^{1/2}$ and that this result is nearly independent of structure and spin. As noted above the latter observation is valid over the entire temperature range and indeed the $(1-T/T_c)^{1/2}$ dependence fits well over the range between $T_c/2$ and T_c (i.e., for values of the reduced magnetization between 0.8 and 0).

In summary, despite the differences in the low-temperature expansions, all four theories are nearly identical in this region, i.e., $kT/Jz<0.1$. For each of the four theories, the curves of the magnetization versus normalized temperature are nearly independent of structure. The Oguchi-Honma theory does indeed give an infinite Curie temperature while the Bloch curve shows the behavior discussed in the previous section: a maximum temperature above which there is no self-consistent solution, but a nonzero magnetization at this temperature. The random phase approximation and Callen theories give definite Curie temperatures.