range of M values for a given G (and vice versa). The measured M is a volume average so that local regions with different values of M and the same G can exist in contact. Since M-H loops exist over a range of temperatures, three or more "phases" are necessary. This explanation of the stability of hysteretic states i.e., the existence of a set of states of differing B with the same free energy implies also that the persistent currents associated with the hysteretic state are stable over a range of values. According to this point of view, the persistent current on the surfaces of hollow cylinders of type-I materials with trapped fields is a manifestation of this same phenomenon. Finally the critical current (and the maximum trapped field) comes about as a result of the system reaching the configuration corresponding to the phase boundary, i.e., it is the value at which G begins to increase. This accounts for the single temperature dependence for t.f.$_{\max}$ observed from different measurements.

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Antiferromagnetically Coupled Impurities in a Heisenberg Ferromagnet*

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The ground state of a ferromagnetic system with an antiferromagnetically coupled impurity is calculated exactly. The spin of the host is arbitrary, as is the ratio of impurity-host exchange to host–host exchange, but the impurity spin is taken to have $S_0=\frac{1}{2}$. The ground-state energy, wave function, spin defect, and critical field for a metamagnetic transition are computed. Results are compared with the approximate spin-wave method as employed by Ishii, Kanamori, and Nakamura. It is shown that the spin-wave method is ambiguous and can lead to grossly incorrect results if applied in particular ways.

I. INTRODUCTION

THE problem of impurity states in magnetic insulators has received much attention recently. Wolfram and Callaway[1] first treated the low-lying eigenstates of a ferromagnet containing a ferromagnetically coupled impurity, applying the rigorous methods of Lifshitz.[2] Recently Ishii, Kanamori, and Nakamura (IKN)[3] have discussed the low-lying eigenstates of a ferromagnet containing an *anti*ferromagnetically coupled impurity, but using an approximate spin-wave analysis. We give here a rigorous theory of this latter problem for arbitrary host spin and exchange interactions, but assuming an impurity spin $S_0=\frac{1}{2}$ and concentrating particularly on the ground-state properties.

The interest in the antiferromagnetically coupled impurity problem is considerably heightened by its close relationship to the problem of the ground state of a pure antiferromagnet.[4] The impurity is found to have a "spin defect" in the ground state (a departure from the pure "spin-down" state of the impurity spin and from the pure "spin-up" state of the host spins). Furthermore, a sharp transition occurs to the wholly aligned state as an external field is applied, in direct analogy to the "metamagnetic transition" in antiferromagnets.[5] As we shall show, both of these effects can be rigorously studied and easily visualized in the impurity problem.

From the purely theoretical point of view, our theory is also of interest because it provides a direct test of the validity of the spin-wave approximation. That method, as used by Ishii, Kanamori, and Nakamura,[3] is a direct transcription of the method introduced by Anderson and commonly applied to the ground state of the antiferromagnet.[4] We shall briefly recapitulate the spin-wave calculation of IKN in Sec. V to compare its results with those of the exact calculation. As we shall see, the method is ambiguous, and differing ways of applying the theory vary from close agreement to marked divergence from the rigorous results.

The third, and presumably not the least, reason for interest in this problem is that the effects here discussed should be observable in real ferromagnetic insulators.

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II. FORMULATION

Consider a Heisenberg ferromagnet with spins of magnitude S and nearest-neighbor positive exchange integral J. The spin at the origin is replaced by an impurity with $S_0=\frac{1}{2}$ and an antiferromagnetic exchange integral $(-\xi J)$

$$\mathcal{H}=-\sum J_{mn}\mathbf{S}_m\cdot\mathbf{S}_n+2\xi J\sum_{\delta}\mathbf{S}_0\cdot\mathbf{S}_\delta, \qquad (1)$$

where neither m nor n may be equal to zero and where $\boldsymbol{\delta}$ is the nearest-neighbor vector, and the sum over $\boldsymbol{\delta}$ ranges over the z neighbors of the impurity.

As the Hamiltonian commutes with $\mathcal{S}^z\equiv\sum_n S_n^z$, we can classify the energy eigenstates by their $\mathcal{S}^z$ eigenvalues. The wholly aligned state is the unique state with maximum $\mathcal{S}^z\equiv\mathcal{S}_0^z$; we shall call this state the "vacuum state." Its wave function is trivially known and its energy is

$$E_v=-NJzS^2+2z(1+\xi/2S)JS^2. \qquad (2)$$

The ground state has $\mathcal{S}^z=\mathcal{S}_0-1$, differing from the vacuum state by a single spin deviation. This characteristic, peculiar to the case of a spin-$\frac{1}{2}$ impurity, is of crucial importance in our analysis.

The Hilbert space of $\mathcal{S}^z=\mathcal{S}_0-1$ is spanned by the local spin deviation states

$$|n\rangle=(2S)^{-1/2}S_n^-\,|\,\text{vac}\rangle, \qquad n\neq 0$$

$$|0\rangle=S_0^-\,|\,\text{vac}\rangle. \qquad (3)$$

These states form a basis in which we consider the matrix elements of $\mathcal{H}$.

The particular states $|n\rangle$ which are centered on the impurity site or on one of its nearest neighbors play a unique role in the theory. We refer to these $z+1$ sites as "the cluster."

We now let $\mathcal{H}=\mathcal{H}_0+V$, defining $\mathcal{H}_0$ as having the same matrix elements as $\mathcal{H}$ (i.e., $\langle n|\mathcal{H}_0|m\rangle=\langle n|\mathcal{H}|m\rangle$) providing neither $|n\rangle$ nor $|m\rangle$ is in the cluster. The matrix elements of $\mathcal{H}_0$ inside the cluster are then defined by imposing spatial translation symmetry. Thus,

$$\langle n|\mathcal{H}_0|m\rangle=[E_v+2zJS]\Delta(n,m)-2JS\Delta(n,m+\delta), \qquad (4)$$

where $\Delta(n,m)$ is unity if $n=m$, and zero otherwise. The matrix elements of V are confined to the cluster, having values only for V_{00}, $V_{0\delta}$, and $V_{\delta\delta}$.

$$\begin{aligned}\langle n|V|m\rangle=&-2z(1+\xi)JS\Delta(n,0)\Delta(m,0)\\&-(2S+\xi)J\Delta(n,\delta)\Delta(m,\delta)\\&+(2S+(2S)^{1/2}\xi)J[\Delta(n,0)\Delta(m,\delta)+\Delta(n,\delta)\Delta(m,0)].\end{aligned} \qquad (5)$$

The single-spin deviation eigenstates of $\mathcal{H}$ are determined by

$$\begin{aligned}(E-\mathcal{H}_0)\,|\psi\rangle\\=V|\psi\rangle=|0\rangle\langle 0|V|\psi\rangle+\sum_\delta|\delta\rangle\langle\delta|V|\psi\rangle,\end{aligned} \qquad (6)$$

where $V|\psi\rangle$ has been expanded in the basis $|n\rangle$, recalling that its matrix elements are restricted to the cluster. Let $|E,n)$ denote the solution of

$$(E-\mathcal{H}_0)\,|E,n)=|n\rangle. \qquad (7)$$

Then the solution of Eq. (6) is

$$\begin{aligned}|\psi\rangle&=|E,0)\,\langle 0|V|\psi\rangle+\sum_\delta|E,\delta)\,\langle\delta|V|\psi\rangle\\&=|E,0)[V_{00}\psi_0+\sum_\delta V_{0\delta}\psi_\delta]\\&\quad+\sum_\delta|E,\delta)[V_{0\delta}\psi_0+V_{\delta\delta}\psi_\delta].\end{aligned} \qquad (8)$$

Multiplying Eq. (8) from the left successively by $\langle 0|$ and by each of the z states $\langle\delta|$ we obtain $(z+1)$ equations in the $(z+1)$ variables ψ_0, ψ_δ. In the ground state all ψ_δ are equal, to be denoted by ψ_1. The $(z+1)$ equations then collapse to 2. The condition that these equations be consistent is found to be

$$1+\xi[(2S+\xi)\epsilon+(2S-1)\xi]^{-1}=2JzS\epsilon G_{00}(\epsilon), \qquad (9)$$

where

$$\epsilon=(E-E_v)/(2JzS) \qquad (10)$$

and $G_{00}(\epsilon)$ denotes the Green's function $\langle 0|E,0)$.

The Green's function $G_{mn}(\epsilon)\equiv\langle m|E,n)$ is easily expressed in terms of the spin-wave eigenvalues of $\mathcal{H}_0$. Denote the spin-wave state of wave vector $\mathbf{k}$ by $|\mathbf{k}\rangle$, and multiply Eq. (7) from the left by $\langle\mathbf{k}|$:

$$\begin{aligned}\langle\mathbf{k}|E,n)&=[2JzS(\epsilon-\epsilon(\mathbf{k}))]^{-1}\langle\mathbf{k}|n\rangle\\&=(2JzSN^{1/2})^{-1}\frac{\exp(-i\mathbf{k}\cdot\mathbf{n})}{\epsilon-\epsilon(\mathbf{k})}.\end{aligned} \qquad (11)$$

In analogy to Eq. (9), $\epsilon(\mathbf{k})$ is the (dimensionless) spin-wave energy of the pure host, in units of $2zJS$. Hence

$$\begin{aligned}G_{mn}(\epsilon)&=\langle m|E,n)=\sum_{\mathbf{k}}\langle m|\mathbf{k}\rangle\langle\mathbf{k}|E,n)\\&=(2zJSN)^{-1}\sum\frac{\exp[i\mathbf{k}\cdot(\mathbf{m}-\mathbf{n})]}{\epsilon-\epsilon(\mathbf{k})}.\end{aligned} \qquad (12)$$

Having the energy ϵ_0 as a root of Eq. (9), the ratio ψ_1/ψ_0 is determined by one of the homogeneous equations obtained from Eq. (8). One easily finds

$$\begin{aligned}\frac{\psi_1}{\psi_0}&=\frac{1-V_{0\delta}/(2JS)-[V_{00}-zV_{0\delta}(\epsilon_0-1)]G_{00}(\epsilon_0)}{V_{\delta\delta}/(2JS)+z[V_{0\delta}-V_{\delta\delta}(\epsilon_0-1)]G_{00}(\epsilon_0)}\\&=(2S)^{1/2}[\epsilon_0/\xi+1].\end{aligned} \qquad (13)$$

Finally, the absolute magnitude of ψ_0 or ψ_1 is determined by combining Eq. (13) with the normalization condition obtained from Eq. (8):

$$1=\langle\psi\mid\psi\rangle=(E,0\mid E,0)[V_{00}\psi_0+zV_{0\delta}\psi_1]^2 +z[(E,\delta\mid E,0)+(E,0\mid E,\delta)] \times[V_{00}\psi_0+zV_{0\delta}\psi_1][V_{0\delta}\psi_0+V_{\delta\delta}\psi_1] +z\sum_{\delta'}(E,\delta\mid E,\delta')[V_{0\delta}\psi_0+V_{\delta\delta}\psi_1]^2. \quad (14)$$

Quantities such as $(E,m\mid E,n)$ are related to derivatives of the Green's function as follows:

$$(E,m\mid E,n)=\langle m\mid(E-\mathcal{H}_0)^{-1}(E-\mathcal{H}_0)^{-1}\mid n\rangle =[(2zJS)^2]^{-1}N^{-1}\sum\frac{\exp[i\mathbf{k}\cdot(\mathbf{n}-\mathbf{m})]}{[\epsilon-\epsilon(\mathbf{k})]^2} =(2zJS)^{-1}(d/d\epsilon)G_{mn}(\epsilon). \quad (15)$$

The Green's functions $G_{mn}(\epsilon)$ for three-dimensional lattices have been tabulated by various authors,[1,6] but most extensively by Mannari and Kawabata.[7]

Having found ψ_0 and ψ_1, the remaining amplitudes $\psi_n=\langle n\mid\psi\rangle$ are found directly from Eq. (8), by multiplying from the left by $\langle n\mid$:

$$\psi_n=\langle n\mid\psi\rangle=(1+\lambda-\lambda\epsilon_0)\psi_0G_{n0}(\epsilon_0), \quad (16)$$

where

$$\lambda=(2S)^{1/2}[\epsilon_0/\xi+1]. \quad (17)$$

Finally various correlation functions can be expressed directly in terms of the amplitudes ψ_n. Of particular interest is the transverse correlation function $\langle\psi\mid S_n^xS_0^x\mid\psi\rangle$ for $n\neq0$. In standard fashion we express S_n^x in terms of S_n^+ and S_n^-

$$\langle\psi\mid S_n^xS_0^x\mid\psi\rangle=\tfrac{1}{4}\langle\psi\mid(S_n^++S_n^-)(S_0^++S_0^-)\mid\psi\rangle =\tfrac{1}{4}\langle\psi\mid S_n^+S_0^-\mid\psi\rangle+\tfrac{1}{4}\langle\psi\mid S_n^-S_0^+\mid\psi\rangle =\tfrac{1}{2}(2S)^{1/2}\psi_n\psi_0. \quad (18)$$

The nearest-neighbor correlation reduces to

$$\langle\psi\mid S_\delta^xS_0^x\mid\psi\rangle=\tfrac{1}{2}(2S)^{1/2}\lambda\psi_0^2 \quad (19)$$

and similarly

$$\langle\psi\mid S_\delta^zS_0^z\mid\psi\rangle=\tfrac{1}{2}S-(S+\tfrac{1}{2}\lambda^2)\psi_0^2. \quad (20)$$

III. RESULTS FOR ZERO EXTERNAL FIELD

Explicit evaluation of the ground-state solution is particularly simple for the linear chain. In that case $G_{00}(\epsilon)$ can be calculated analytically:

$$G_{00}(\epsilon)=(4JS)^{-1}\pi^{-1}\int_0^\pi[\epsilon-1+\cos k]^{-1}dk =\frac{-1}{4JS}(\epsilon^2-2\epsilon)^{-1/2}. \quad (21)$$

If we choose $\xi=1$ and $S=\frac{1}{2}$, we find, from Eq. (9),

$$\epsilon_0=-\tfrac{1}{8}(7+\sqrt{17})=-1.3904, \quad (22)$$

whence, from Eq. (13),

$$\psi_1/\psi_0=-0.3904. \quad (23)$$

Then, from Eq. (14)

$$\psi_0^2=0.7570, \quad (24)$$

and Δ, the spin defect on the impurity spin, is

$$\Delta=1-\psi_0^2=0.243. \quad (25)$$

The ground-state wave function is explicitly given by Eq. (16). In Fig. 1, we plot the wave function for a one-dimensional chain with $2S=\xi=1$; the general shape is similar for other values of the parameters. It should be noted that the wave function changes sign between the impurity and its neighbors, implying [in accordance with Eq. (19)] that the transverse spin components are antiparallel. This negative correlation function is clearly to be expected on the basis of the antiferromagnetic coupling of impurity to host spins.

In two dimensions, the Green's function can again be calculated analytically, in terms of complete elliptic integral. For $z=4$, $\xi=1$, and $S=\frac{1}{2}$, we find $\Delta=0.106$ and $\epsilon_0=-1.17$.

In three dimensions we have computed the Green's function by using the expansion coefficients given in Ref. (7). In Fig. 2 we plot the ground-state energy as a function of the ratio ξ of exchange integrals, for various

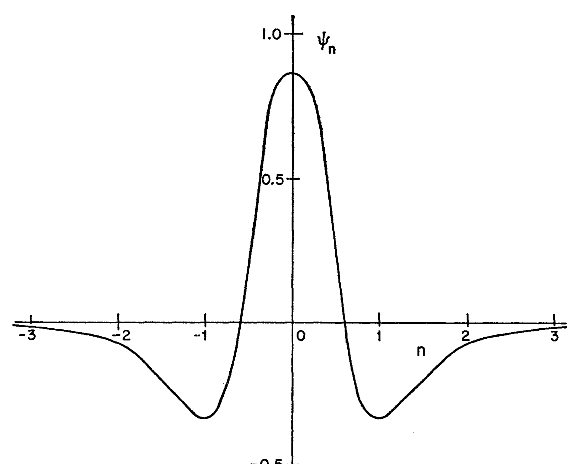

FIG. 1. Ground-state wave function for linear chain ($2S=\xi=1$, $H=0$).

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values of the host spin. Each curve is *almost* linear, but with a slight upward concavity; for large ξ they become straight lines with

$$-\epsilon_0 \simeq (1+1/2zS)\xi, \qquad \xi \gg 1. \tag{26}$$

In Fig. 3 we give the corresponding spin defect of the impurity. The spin defect increases with increasing ξ, tending to the limit

$$\Delta \to (2zS+1)^{-1} \qquad \text{as } \xi \to \infty. \tag{27}$$

IV. EXTERNAL MAGNETIC FIELD, AND THE METAMAGNETIC TRANSITION

We now consider the effect of an external magnetic field, applied along the z direction. Suppose first that the g factors of the impurity and the host spins are the same. The only effect then is to shift the ground-state energy by $g\mu_B H$, with no effect on the wave function. This follows by noting that each state $|n\rangle$ is increased in energy by $g\mu_B H$, whence every linear combination of the states $|n\rangle$ is similarly affected. Or, more formally, the perturbing potential V of Eq. (5) is independent of H, whereas the Green's functions G_{mn} are altered merely by $\epsilon \to \epsilon + g\mu_B H/(2zJS)$. The consequent increase in the energy of the ground state (relative to the fully aligned "vacuum" state) eventually raises its energy above the vacuum. There is then an abrupt change in the physical ground state, from the state with $\mathcal{S}^z = \mathcal{S}_0 - 1$ to the fully aligned state $\mathcal{S}_0$.

The critical field H_c for the "metamagnetic transition" is then

$$g\mu_B H_c = -\epsilon_0(2JzS), \tag{28}$$

where ϵ_0 is the energy of the ground state in the absence of the field, as given by Eq. (9) or Fig. 2.

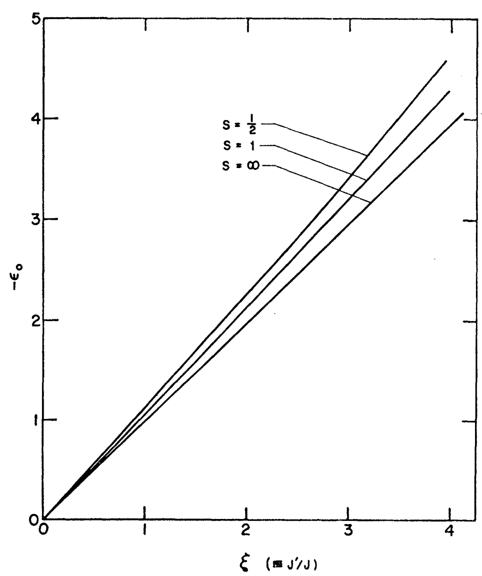

FIG. 2. Ground-state energy (simple cubic lattice, $H=0$).

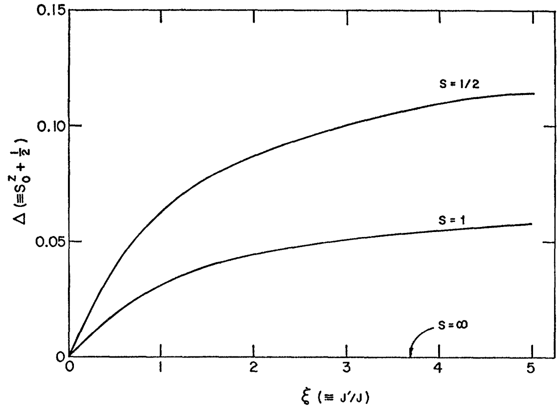

FIG. 3. Spin defect of the impurity spin (simple cubic lattice, $H=0$).

In the more general case, in which the g factors of impurity and host differ, the formalism is again easily generalized. Let g' be the g factor of the impurity, and g be that of the host. Then the previously given formalism is altered only by the addition of the term $(g'-g)\mu_B H$ to V_{00} and by the replacement of ϵ by $\epsilon - g\mu_B H/(2JzS)$ in the argument of the Green's functions. The energy equation, analogous to Eq. (9) is

$$\frac{1}{\epsilon'}\left\{1+\frac{\xi(\epsilon'-\eta)}{(2S+\xi)\epsilon'^2+(2S-1)\xi\epsilon'-[(2S+\xi)\epsilon'-\xi]\eta}\right\} = (2JzS)G_{00}(\epsilon'), \tag{29}$$

where

$$\epsilon' = \epsilon - g\mu_B h, \tag{30}$$

$$\eta = (g'-g)\mu_B h, \tag{31}$$

and

$$h = H/(2JzS). \tag{32}$$

In contrast to the case $g'=g$, the magnetic field now alters the wave function. If $g'>g$ the field tends to increase the spin defect on the impurity. These effects are shown in Fig. 4 in which we plot the spin defect on the impurity as a function of applied field for various values of g'/g; we have again taken a simple cubic array with $\xi = 2S = 1$. The effect is also evident in Fig. 5, in which we plot the energy of the nominal ground state as a function of magnetic field.

The critical field for the metamagnetic transition is readily obtained as the zero of the energy curve of Fig. 5. Or, stated equivalently, it is obtained by solving Eq. (29) for h, after taking $\epsilon' = -g\mu_B h$ (or $\epsilon = 0$). Figure 6 illustrates the dependence of critical field on g'/g, for the case of $2S = \xi = 1$.

Although we have inferred the ground state by comparing the energy of the vacuum state and the ground state of $\mathcal{S}^z = \mathcal{S}_0 - 1$, it must be recalled that under special circumstances (such as $g' \gg g$ and $\xi \gg 1$), other states may compete and must be considered also.

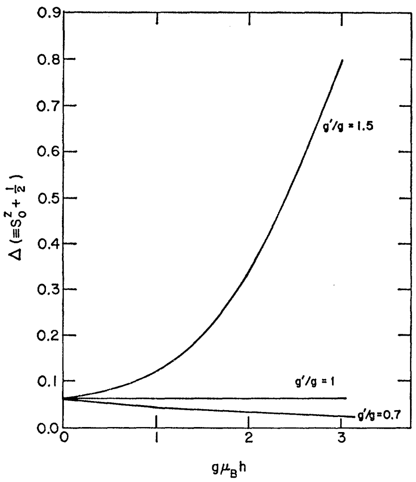

FIG. 4. Spin defect of impurity, as a function of external field (simple cubic, $2S=\xi=1$).

V. THE SPIN-WAVE APPROXIMATION

For purposes of comparison we briefly recapitulate the spin-wave method of IKN. The procedure is as follows. One first introduces the local boson operators by the usual transformation (but note the inversion of definition for the impurity site):

$$a_n{}^{+}=(2S)^{-1/2}S_n{}^{-}, \qquad n\neq 0$$
$$=S_0{}^{+}, \qquad n=0. \tag{33}$$

This step is, of course, the fateful one in the spin-wave procedure. The boson operator $a_n{}^{\dagger}$ has the correct matrix element between the spin-up state and the single spin deviation state at site $n(n\neq 0)$, whereas all other matrix elements are incorrect. At the impurity site, $a_0{}^{\dagger}$ has the correct matrix element between the spin-down state and the state of a single flip up; again all other matrix elements are incorrect, even to the extent of allowing an infinite number of flips up at the impurity site. (These erroneous matrix elements are, of course, most severe when the impurity spin has $S_0=\frac{1}{2}$.) Thus the transformation (33) is predicated on the ground state being very close to the Néel state.

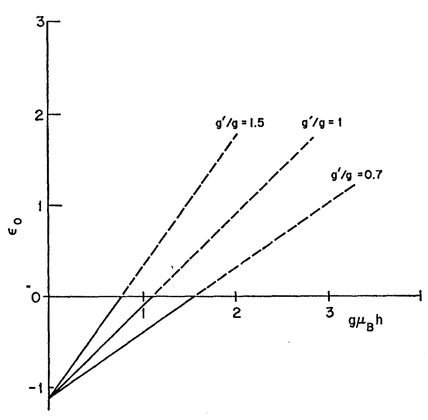

FIG. 5. Ground-state energy as a function of external field (simple cubic, $2S=\xi=1$).

The second step of the spin-wave approximation consists of seeking operators c_q of the form

$$c_q=\Gamma_0{}^q a_0{}^{\dagger}+\sum_{n\neq 0}\Gamma_n{}^q a_n, \tag{34}$$

which satisfy the commutation relation

$$[c_q,\mathcal{H}]=\epsilon_q c_q. \tag{35}$$

Of course the adjoint operator $c_q{}^{\dagger}$ then creates an excitation of energy ϵ_q; in the pure ferromagnet or antiferromagnet these excitations are spin waves, but in the impurity problem the excitations may be localized modes (in which case q loses its significance as a wave vector).

Making the transformation (33) in the Hamiltonian and retaining only quadratic terms, one finds[3] that the $\Gamma_n{}^q$ are uniquely determined by Eq. (35).

One particular mode so found (which IKN designate the "s_0 mode") has negative energy. The interpretation

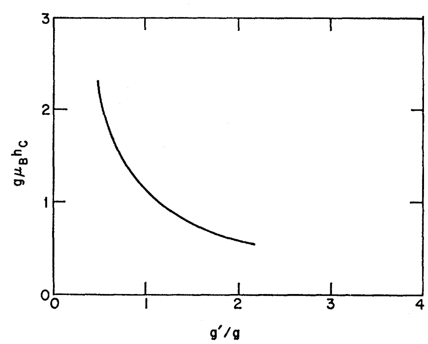

FIG. 6. Critical field for "metamagnetic" transition (simple cubic, $2S=\xi=1$).

of this result is that the "creation operator" $c_s{}^{\dagger}$ is actually a destruction operator. Whereas for every other mode the creation operator decreases $\mathcal{S}^z$ by one unit [see Eqs. (33) and (34)], for this unique mode the creation operator increases $\mathcal{S}^z$. If the ground state has $\mathcal{S}^z=\mathcal{S}_0-1$, then the s_0 mode has $\mathcal{S}^z=\mathcal{S}_0$, whereas all other modes created by the $c_q{}^{\dagger}$ have $\mathcal{S}^z=\mathcal{S}_0-2$. Consequently *the* s_0 *mode of* IKN *is identical with the vacuum state.*

The energy of the s_0 mode is the energy of the vacuum state relative to the ground state. If ϵ_s is the dimensionless energy of the s_0 mode, and ϵ_v is the dimensionless energy of the vacuum state [see Eq. (2)] then the ground-state energy ϵ_{ground} is

$$\epsilon_{\text{ground}}=\epsilon_v-\epsilon_s. \tag{36}$$

Similarly the ground-state wave function follows immediately:

$$|\,\text{ground}\rangle=c_s\,|\,\text{vac}\rangle, \tag{37}$$

where c_s is now the *destruction* operator of the s_0 mode.

Although the above procedure is simple and direct, the results are distressing. For example the ground-state energy for a linear chain with $2S=\xi=1$ is $\epsilon_v-0.67$. For a three-dimensional simple cubic array with $2S=\xi=1$, the ground-state energy is $\epsilon_v-0.905$. In each of these cases the Néel state has energy $\epsilon_v-1.00$. Hence the ground-state energy is predicted to be higher than the Néel state!

The wave function obtained in this fashion is similarly poor. In fact it shows no nodes, as contrasted with the sign inversion of the true wave function as shown in Fig. 1. Consequently the transverse components of the nearest-neighbor spins are parallel to the impurity spin, rather than antiparallel! It is this incorrect correlation which raises the ground-state energy above the Néel energy.

Despite the poor results above, there is an alternative way to infer the ground state from the spin-wave approximation. Inverting Eq. (34) and expressing the Hamiltonian in terms of the c_q and $c_q{}^\dagger$ operators, one finds

$$(2zJS)^{-1}\mathcal{H}=\epsilon_{\text{ground}}+\sum_q \epsilon_q c_q{}^\dagger c_q \tag{38}$$

where, for $2S=\xi=1$,

$$\epsilon_{\text{ground}}=\epsilon_v-1+2[|\Gamma_0{}^0|^2-1-\tfrac{1}{2}z^{-1}\sum\Gamma_n{}^{0*}\Gamma_{n+\delta}{}^0]. \tag{39}$$

The summation can be simplified in terms of Green's functions and their derivatives. Using the values of $\Gamma_n{}^0$ found by IKN,[3]

$$\sum_{n,\delta}\Gamma_n{}^{0*}\Gamma_{n+\delta}{}^0=|A_0|^2\sum_{n,\delta}G_{n0}{}^*G_{n+\delta,0}$$
$$=|A_0|^2[(\epsilon_s-1)(dG_{00}/d\epsilon_s)+G_{00}]/(2JS), \tag{40}$$

where

$$|A_0|^2=[2G_{00}{}^2+(2JzS)^{-1}(dG_{00}/d\epsilon_s)]^{-1}. \tag{41}$$

Numerical calculation gives the ground-state energy relative to the vacuum-state energy for the linear chain with $2S=\xi=1$,

$$\epsilon_0=-1.333 \quad \text{(spin-wave approx.)} \tag{42}$$

which is to be compared with the rigorous result

$$\epsilon_0=-1.3904. \tag{43}$$

For the simple cubic array with $2S=\xi=1$,

$$\epsilon_0=-1.084 \quad \text{(spin-wave approx.)}, \tag{44}$$

whereas the rigorous result is

$$\epsilon_0=-1.1015. \tag{45}$$

Thus this way of applying the spin-wave approximation gives results which are quite accurate (within a few percent).

Comparable accuracy is obtained for the spin defects of the impurity spin. For $2S=\xi=1$ the spin-wave approximation gives

$$\Delta=0.333 \quad \text{(linear chain, spin-wave approx.)},$$
$$\Delta=0.112 \quad \text{(square array, spin-wave approx.)},$$
$$\Delta=0.062 \quad \text{(cubic array, spin-wave approx.)}, \tag{46}$$

whereas the rigorous results are

$$\Delta=0.243 \quad \text{(linear chain, exact)},$$
$$\Delta=0.106 \quad \text{(square array, exact)},$$
$$\Delta=0.062 \quad \text{(cubic array, exact)}. \tag{47}$$

Although the error is $\sim 30\%$ for the linear chain it is negligible in three dimensions.

Comparison of the two methods of applying the spin-wave approximation indicates that this approximation is more reliable for the ground state than for the excited states. The s_0 mode is particularly poorly given. In the first method of applying the approximation we inferred properties of the ground state from the known properties of the s_0 mode, thereby transferring the calculational inaccuracies of that mode back to the ground state. Fortunately the usual method of applying the spin-wave approximation in antiferromagnets is closely akin to the second type of calculation above. Nevertheless it would seem that the internal inconsistency exhibited here stresses the need for caution.

ACKNOWLEDGMENTS

We are indebted to Professor J. Kanamori for an instructive commentary on the spin-wave calculation of the vacuum state (or s_0 mode), and to Professor Daniel Hone for several illuminating discussions.