Bound States of Two Spin Waves in the Heisenberg Ferromagnet

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The simple cubic nearest-neighbor Heisenberg model is discussed in one, two, and three dimensions for arbitrary spin. The problem of two spin deviations propagating in an otherwise fully aligned lattice is reduced to quadratures. The integrals relevant to the bound-state problem are examined. It is found that bound states exist for all spins and dimensionalities. In one dimension the results of Bethe and others are reaffirmed. In two and three dimensions the total momentum of a bound pair determines the number of possible bound states. For positive exchange constant and sufficiently large longitudinal anisotropy there are bound states of two spin waves with energies below all continuum energies. It is argued that these states should have a dominant influence on the low-temperature thermodynamics.

1. INTRODUCTION

THE Heisenberg Hamiltonian conserves the component of total spin along the direction of the external magnetic field. The set of states of the system having an eigenvalue of this component of the total spin differing by a given integer, n, from the totally aligned value comprise an invariant subspace under the dynamical motion. The quantum number, n, labels the number of spin deviations or spin waves in the system.

The $n=0$ subspace contains a single state. Bloch[1] showed that the $n=1$ subspace is diagonalized by a momentum representation. The $n=2$ subspace is the first to exhibit effects of spin wave–spin wave interactions. For a one-dimensional lattice and spin $S=\frac{1}{2}$ Bethe[2] solved the resulting two-particle problem completely. He found that in the limit as the lattice becomes large there exists a unique bound state for each value $\mathbf{K}$ of the total momentum of the pair. He did not extend his treatment to higher dimensionalities. Van Kranendonk[3] was the first to attack the more general problem; however, unable to carry through the calculation exactly, he was forced to introduce approximations which misrepresented the dynamics of the spin system and led to erroneous results. The two-particle problem has been discussed more recently by Dyson[4] as a part of his monumental calculation of the low-temperature thermodynamics of the Heisenberg model. Dyson derived a bound-state condition valid at $\mathbf{K}=0$. He verified in two and three dimensions and for arbitrary S that this condition is not fulfilled and went on to conjecture that bound states fail to exist for all $\mathbf{K}$. We shall show below that this conjecture is false. In two dimensions, because of the very singular behavior of the relevant integrals at $\mathbf{K}=0$, there exist bound states for arbitrarily small nonzero $\mathbf{K}$. In three dimensions there is, indeed, a region of small $\mathbf{K}$ for which bound states are absent; however, as $\mathbf{K}$ increases in magnitude, a threshold is reached above which they appear.

The program of the present paper is to reduce the two-particle problem to quadratures without approximation, to pick out a bound-state condition valid for arbitrary $\mathbf{K}$, and to analyze this condition successively in one, two, and three dimensions. In one dimension Bethe's[2] results are rederived for arbitrary spin. In two and three dimensions contact is made with Dyson's discussion, as mentioned above. In a final section a longitudinal anisotropy is incorporated into the Hamiltonian and the problems associated with experimental observation of the two-spin-wave bound states are briefly discussed.

2. FORMULATION OF THE PROBLEM

Consider a finite, cubic array of points, $\mathbf{R}_i$, which may be thought of as the vertices of a lattice of unit spacing[5] and side L. It is convenient to assume that the lattice has periodic connectivity, i.e., that the point $(\mathbf{R}_i+L\mathbf{R}_j)$ is identical with the point $\mathbf{R}_i$ for all $\mathbf{R}_i$ and $\mathbf{R}_j$ lattice vectors. Thus, there are no edge effects and all lattice sites are perfectly equivalent. There are a total of $N=L^d$ lattice points, where d is the lattice dimensionality. In the formalism to be described below it will prove compact to let a numerical argument stand for a general lattice point.

A spin, $\mathbf{S}(1)$, of magnitude S is associated with each lattice point. These spins satisfy (in units such that $\hbar=1$, which will be used throughout) the usual relations,

$$[S^{\pm}(1),S^{z}(2)]=\mp\delta(12)S^{\pm}(2), \tag{1}$$

$$[S^{-}(1),S^{+}(2)]=-2\delta(12)S^{z}(2), \tag{2}$$

$$S^{+}(1)S^{-}(1)+S^{z}(1)[S^{z}(1)-1]=S(S+1), \tag{3}$$

and

$$[S^{+}(1)]^{2S+1}=[S^{-}(1)]^{2S+1}=0, \tag{4}$$

where

$$S^{\pm}(1)=S^{x}(1)\pm iS^{y}(1), \tag{5}$$

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[2] H. A. Bethe, Z. Physik **71**, 205 (1931); A. Sommerfeld and H. A. Bethe, in *Handbuch der Physik*, edited by H. Geiger and Karl Scheel (Julius Springer-Verlag, Berlin, 1933), Vol. 24, Part 2, pp. 604–618.

[3] J. Van Kranendonk, Physica **21**, 749 (1955).

[4] F. J. Dyson, Phys. Rev. **102**, 1217 (1956).

[5] Since the Heisenberg problem consists entirely of spins and has no spatial dynamics, the actual size of the lattice spacing enters the model only through the parameters of the spin-spin interaction.

and the arguments, 1 and 2, refer to general lattice points. The space of states of the Heisenberg model is the direct product over all lattice sites of the individual spin state spaces.

The dynamics of the Heisenberg model is governed by the Hamiltonian

$$H=\mu\sum_1 S^z(1)-\tfrac{1}{2}\sum_{1,2} J(12)\mathbf{S}(1)\cdot\mathbf{S}(2). \tag{6}$$

The first term represents the interaction of each spin with a time-independent, spatially homogeneous external magnetic field, the direction of which has been chosen as the z axis. The letter μ stands for the product of the spin magnetic moment and the magnitude of the external field. The second term is an isotropic nearest neighbor exchange interaction,

$$\begin{aligned} J(12)=J(21)&=J \quad \text{for} \quad 1 \text{ and } 2 \text{ nearest neighbors} \\ &=0 \qquad\quad \text{otherwise}. \end{aligned} \tag{7}$$

When $J>0$ (<0) the system is ferromagnetic (antiferromagnetic) at low temperatures. The summations are carried out over all lattice sites.

It is straightforward to verify that the spin deviation number operator,

$$n=NS+\sum_1 S^z(1), \tag{8}$$

commutes with H. The unique state with $n=0$, which we shall designate by $|0\rangle$ (normalized), is an eigenstate[6] of H with energy

$$E_0=-\mu NS-dNJS^2. \tag{9}$$

The state $|0\rangle$ is totally aligned:

$$S^z(1)|0\rangle=-S|0\rangle. \tag{10}$$

When $J>0$ and $\mu>0$, $|0\rangle$ is the ground state of the Hamiltonian (6). Only under these conditions are the states of small n of particular thermodynamical importance. The normalized states of the $n=1$ and $n=2$ subspaces are now simply generated from $|0\rangle$:

$$S^+(1)|0\rangle=[(2S)]^{1/2}|1\rangle, \tag{11}$$

$$S^+(1)S^+(2)|0\rangle=[(2S)^2(1+\delta(12))h_2(12)]^{1/2}|12\rangle, \tag{12}$$

where

$$h_2(12)=[1-\delta(12)/2S]. \tag{13}$$

Here the notation $|1\cdots\rangle$ stands for a normalized state in which a unit of spin has been flipped away from total alignment on each of the sites $1, \cdots$. The normalization factors can be computed from the commutation relations. Note that $h_2(11)=0$ for $S=\frac{1}{2}$.

Define now the one- and two-particle Green's functions,

$$G_1(1;1';t)=(-i)\langle 0|S^-(1;t)S^+(1';0)|0\rangle\eta(t), \tag{14}$$

$$\begin{aligned} G_2(12;1'2';t)=(-i)^2\langle 0|S^-(1;t)S^-(2;t) \\ \times S^+(1';0)S^+(2';0)|0\rangle\eta(t), \end{aligned} \tag{15}$$

where

$$\begin{aligned} \eta(t)&=1, \quad t>0 \\ &=0, \quad t<0. \end{aligned} \tag{16}$$

The standard Heisenberg time development is taken:

$$\mathbf{S}(1;t)\equiv e^{iHt}\mathbf{S}(1;0)e^{-iHt}. \tag{17}$$

In what follows the time argument will frequently be omitted. The appearance of the η function implies the boundary condition,

$$G_1(\cdots;t)=G_2(\cdots;t)=0, \quad \text{when} \quad t<0. \tag{18}$$

It is instructive to exhibit explicitly the relation between the Green's functions and the one- and two-particle wave functions and matrix elements of the Heisenberg model. The Fourier transform of G_n, defined by

$$G_n(\cdots;t)=i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}G_n(\cdots;\omega), \tag{19}$$

has the form

$$\begin{aligned} &G_n(1\cdots;1'\cdots;\omega) \\ &=(-i)^n\sum_\gamma\frac{\langle 0|S^-(1)\cdots|\gamma\rangle\langle\gamma|S^+(1')\cdots|0\rangle}{(\omega-(E_\gamma-E_0)+i\epsilon)}, \end{aligned} \tag{20}$$

where all operators are taken at $t=0$ and the $|\gamma\rangle$ are a complete orthonormal set of n-particle energy eigenstates. The $i\epsilon$ standing in the denominator is intended to suggest the operation $\lim_{0<\epsilon\to 0}$ and incorporates the boundary condition (18). The matrix elements in the numerator of (20) can be expressed as

$$\langle 0|S^-(1)|\gamma\rangle=[2S]^{1/2}\psi_\gamma(1)=[2S]^{1/2}\langle 1|\gamma\rangle \tag{21}$$

and

$$\begin{aligned} \langle 0|S^-(1)S^-(2)|\gamma\rangle&=[(2S)^2h_2(12)]^{1/2}\psi_\gamma(12) \\ &=[(2S)^2(1+\delta(12))h_2(12)]^{1/2}\langle 12|\gamma\rangle. \end{aligned} \tag{22}$$

When $S=\frac{1}{2}$, Eq. (22) does not define the nonexistent wave function $\psi_\gamma(11)$. The wave functions are orthonormal according to

$$\sum_{1\cdots}{}'\psi_\gamma^\dagger(1\cdots)\psi_{\gamma'}(1\cdots)=n!\delta(\gamma\gamma'), \tag{23}$$

where the prime indicates summation only over physically meaningful wave functions. The completeness relations are

$$\sum_\gamma\psi_\gamma^\dagger(1')\psi_\gamma(1)=\delta(11') \tag{24}$$

[6] Note that there is perfect symmetry with respect to the orientation of the z axis parallel or antiparallel to the magnetic field. The transformation $S^z(1)\to -S^z(1)$, $S^+(1)\leftrightarrow S^-(1)$ preserves the relations (1)–(4) and is equivalent in the Hamiltonian (6) to the change, $\mu\to-\mu$. We might in place of (8) have used the definition, $n'=NS-\sum_1 S^z(1)$, and proceeded to work away from the unique state $n'=0$ ($n=2SN$); however, the results would be entirely equivalent to using (8) with the sign of μ reversed.

and

$$\sum_\gamma \psi_\gamma^\dagger(1'2')\psi_\gamma(12)=\delta(11')\delta(22')+\delta(12')\delta(21'). \quad (25)$$

Equations (19)–(22) show that the functions G_1 and G_2 contain all possible information about the one- and two-particle subspaces. In what follows we shall compute G_2 by using its equation of motion, the boundary condition (18), and spatial periodicity, which takes the form

$$G_n(\cdots\mathbf{R}_i\cdots;t)=G_n(\cdots\mathbf{R}_i+L\mathbf{R}_j\cdots;t), \quad \mathbf{R}_i \text{ and } \mathbf{R}_j \text{ lattice vectors.} \quad (26)$$

Before embarking on the full G_2 problem, let us illustrate the method by constructing the function G_1, which will be a convenient auxiliary in later calculation.

The equation of motion for $S^-(1)$ following from the Hamiltonian (6) is

$$\left(i\frac{\partial}{\partial t}-\mu\right)S^-(1) + \sum_{\bar{1}} J(1\bar{1})[S^z(\bar{1})S^-(1)-S^z(1)S^-(\bar{1})]=0. \quad (27)$$

Equation (27) and the property (10) of the state $|0\rangle$ imply an equation of motion for G_1:

$$\left(i\frac{\partial}{\partial t}-\mu\right)G_1(1;1') - S\sum_{\bar{1}} J(1\bar{1})[G_1(1;1')-G_1(\bar{1};1')] = \delta(t)\langle 0|[S^-(1),S^+(1')]|0\rangle = 2S\delta(t)\delta(11'). \quad (28)$$

The equivalence of the lattice points guarantees that $G_1(1;1')$ can only depend on the coordinate difference $(1-1')$. The periodicity requirement (26) is incorporated by expressing G_1 as a spatial Fourier series with respect to the $\mathbf{k}$ vectors of the reciprocal lattice. Once spatial and temporal transforms are taken, Eq. (28) is trivially soluble and the result is

$$G_1(1;1')=\frac{2S}{N}\sum_{\mathbf{k}\epsilon F} e^{i\mathbf{k}\cdot(1-1')}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{e^{-it\omega}}{(\omega-\mu-\Omega(\mathbf{k})+i\epsilon)}, \quad (29)$$

where

$$\Omega(\mathbf{k})=2SJ\sum_{i=1}^{d}(1-\cos k_i). \quad (30)$$

The sum in (29) is over the set F containing the reciprocal lattice vectors with components

$$k_i=(2\pi/L)m_i, \quad i=1,\cdots,d$$
$$m_i \text{ integral: } -(\tfrac{1}{2}L-1)\leqslant m_i\leqslant \tfrac{1}{2}L, \quad L \text{ even}$$
$$-(\tfrac{1}{2}L-\tfrac{1}{2})\leqslant m_i\leqslant(\tfrac{1}{2}L-\tfrac{1}{2}), \quad L \text{ odd.} \quad (31)$$

Clearly, $G_1(1;1')$ has just the form of (20). The spectrum (30) is just that derived by Bloch[1] for single spin waves in an otherwise aligned lattice.

3. SOLUTION OF THE TWO-PARTICLE PROBLEM

We are now in a position to calculate G_2. The equation of motion for the combination $S^-(1)S^-(2)$ can be caclulated from (27); however, in writing an equation of motion for G_2 the S^z's resulting from the differentiation of $S^-(2)$ must be commuted through $S^-(1)$ to the left, so they can project onto $\langle 0|$ according to (10). The equation of motion obeyed by G_2 is

$$\left[i\frac{\partial}{\partial t}-2(\mu+2SdJ)\right]G_2(12;1'2') + S\sum_{\bar{1}} J(1\bar{1})G_2(\bar{1}2;1'2') + S\sum_{\bar{2}} J(2\bar{2})G_2(1\bar{2};1'2') + J(12)G_2(12;1'2') - \delta(12)\sum_{\bar{1}} J(1\bar{1})G_2(\bar{1}2;1'2') = (-i)(2S)^2[\delta(11')\delta(22')+\delta(12')\delta(21')]h_2(1'2'). \quad (32)$$

The last two terms on the left-hand side of this equation are a consequence of the commutation process described above. They make explicit reference to both the position 1 and the position 2 and may be regarded as interactions between particles whose free motion is described by the three preceding terms. To exploit this analogy, introduce the symmetrical function

$$\Gamma_2(12;1'2';t)\equiv G_1(1;1')G_1(2;2') + G_1(1;2')G_1(2;1'). \quad (33)$$

It can be verified directly that $\Gamma_2(12;1'2')$ satisfies Eq. (32) with the interaction terms omitted from the left side and the factor $h_2(1'2')$ omitted from the right. With the help of Γ_2 the equation of motion (32) may now be transformed into an integral equation, which incorporates the boundary conditions through the structure of G_1:

$$G_2(12;1'2';t)=\Gamma_2(12;1'2';t)h_2(1'2') - \frac{i}{2(2S)^2}\sum_{\bar{1}\bar{2}}\int_{-\infty}^{\infty}d\bar{t}K_2(12;\bar{1}\bar{2};t-\bar{t})J(\bar{1}\bar{2}) \times G_2(\bar{1}\bar{2};1'2';\bar{t}), \quad (34)$$

where

$$K_2(12;\bar{1}\bar{2})=\Gamma_2(12;\bar{1}\bar{2}) - \tfrac{1}{2}[\Gamma_2(12;\bar{1}\bar{1})+\Gamma_2(12;\bar{2}\bar{2})] \quad (35)$$

and the symmetry of G_2 in its unprimed arguments has been invoked. Note the asymmetry between primed

and unprimed coordinates in Eq. (34).[7] Had we used instead of (32) the corresponding equation for the primed indices, the analog of (34) would have had the opposite asymmetry. The asymmetry seems to be an unavoidable consequence of the spin commutation relation (2).

Equation (34) can be solved by Fourier transformation. Sum and difference variables are introduced according to

$$2\mathbf{R}=1+2, \quad \mathbf{r}=1-2$$
$$\text{and} \tag{36}$$
$$\mathbf{K}=\mathbf{k}_1+\mathbf{k}_2, \quad 2\mathbf{k}=\mathbf{k}_1-\mathbf{k}_2.$$

Equations (29), (33), and (35) may be combined to give

$$\Gamma_2(12;1'2')=\frac{1}{N}\sum_{\mathbf{K}\epsilon F} e^{i\mathbf{K}\cdot(\mathbf{R}-\mathbf{R}')} \times i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}\Gamma_2(\mathbf{r};\mathbf{r}';\mathbf{K},\omega) \tag{37}$$

and

$$K_2(12;1'2')=\frac{1}{N}\sum_{\mathbf{K}\epsilon F} e^{i\mathbf{K}\cdot(\mathbf{R}-\mathbf{R}')} \times i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}K_2(\mathbf{r};\mathbf{r}';\mathbf{K},\omega), \tag{38}$$

with

$$\Gamma_2(\mathbf{r};\mathbf{r}';\mathbf{K},\omega)=\frac{(-2)(2S)^2}{N}\sum_{\mathbf{k}\epsilon\bar{F}}\frac{\cos\mathbf{k}\cdot\mathbf{r}\,\cos\mathbf{k}\cdot\mathbf{r}'}{\omega-2\mu-S(\mathbf{k},\mathbf{K})+i\epsilon} \tag{39}$$

and

$$K_2(\mathbf{r};\mathbf{r}';\mathbf{K},\omega)=\frac{(-2)(2S)^2}{N} \times\sum_{\mathbf{k}\epsilon\bar{F}}\frac{\cos\mathbf{k}\cdot\mathbf{r}[\cos\mathbf{k}\cdot\mathbf{r}'-\cos\tfrac{1}{2}\mathbf{K}\cdot\mathbf{r}']}{\omega-2\mu-S(\mathbf{k},\mathbf{K})+i\epsilon}, \tag{40}$$

where

$$S(\mathbf{k},\mathbf{K})=\Omega(\mathbf{k}_1)+\Omega(\mathbf{k}_2) =4SJ\textstyle\sum_i(1-\cos\frac{1}{2}K_i\cos k_i), \tag{41}$$

and $\bar{F}$ denotes the set of modified reciprocal lattice vectors with components:

$$2k_i=(2\pi/L)m_i, \quad i=1,\cdots,d$$
$$-(L-2)\leqslant m_i\leqslant L \quad \text{for } L \text{ and } LK_i/2\pi \text{ same parity}, \tag{42}$$
$$-(L-1)\leqslant m_i\leqslant (L-1) \quad \text{for } L \text{ and } LK_i/2\pi \text{ opposite parity}.$$

[7] For example, the $S=\frac{1}{2}$ property, $G_2(12;1'1')=0$, which follows from (4), is clearly a property of the integral equation (34), through the appearance of the factor $h_2(1'2')$. The corresponding property for the unprimed coordinates, $G_2(11;1'2')=0$, is not manifest in (34) and depends on a complicated cancellation between the "free" term and the "scattering" term. This property does follow directly from the differential equation (32), due to a cancellation between the second, third, and fifth terms on the left-hand side.

m_i is integral and goes by steps of two between the limits shown. Now, G_2 can only depend on the coordinate differences $\mathbf{r}$, $\mathbf{r}'$, and $(\mathbf{R}-\mathbf{R}')$. For fixed $\mathbf{r}$ and $\mathbf{r}'$ the variable $(\mathbf{R}-\mathbf{R}')$ has the periodicity of the lattice, so G_2 can be represented as

$$G_2(12;1'2')=\frac{1}{N}\sum_{\mathbf{K}\epsilon F} e^{i\mathbf{K}\cdot(\mathbf{R}-\mathbf{R}')}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t} \times G_2(\mathbf{r};\mathbf{r}';\mathbf{K},\omega). \tag{43}$$

The symmetry of G_2 in 1, 2, and in $1'$, $2'$ requires that $G_2(\mathbf{r};\mathbf{r}';\mathbf{K},\omega)$ be even in $\mathbf{r}$ and $\mathbf{r}'$.

When the representations (37), (38), and (43) are substituted into (34), one finds

$$G_2(\mathbf{r};\mathbf{r}';\mathbf{K},\omega)=\Gamma_2(\mathbf{r};\mathbf{r}';\mathbf{K},\omega)h_2(\mathbf{r}') +\frac{J}{(2S)^2}\sum_j K_2(\mathbf{r};j;\mathbf{K},\omega)G_2(j;\mathbf{r}';\mathbf{K},\omega), \tag{44}$$

where j denotes a unit lattice vector and ranges over the d spatial directions. If $\mathbf{r}$ is replaced by a unit lattice vector i, Eq. (44) becomes for each $\mathbf{r}'$, $\mathbf{K}$, and ω a set of d equations in the d unknowns $G_2(i;\mathbf{r}';\mathbf{K},\omega)$. By reinserting the solution on the right-hand side of (44), we may then compute the full $G_2(\mathbf{r};\mathbf{r}';\mathbf{K},\omega)$, from which the wave functions, energy eigenvalues, etc. follow by (43), (20), and (22). For general L and $\mathbf{K}$ the difficulty of performing exactly the summations (39) and (40) makes this full program unfeasible.[8]

It is useful, however, to analyze further the structure of the function $G_2(\mathbf{r};\mathbf{r}';\mathbf{K},\omega)$ as a function of its energy variable, ω. If we choose to regard ω as a complex variable, $\omega\rightarrow z$, the representation (20) shows that the poles of $G_2(\mathbf{r};\mathbf{r}';\mathbf{K},z)$ as a function of z lie on the real z axis at values given by the differences between the two-spin-wave eigenenergies and E_0. Formulas (39) and (40) show that the functions $\Gamma_2(\mathbf{r};\mathbf{r}';\mathbf{K},z)$ and $K_2(\mathbf{r};\mathbf{r}';\mathbf{K},z)$ have poles at the energies (relative to E_0) of two noninteracting spin waves and are otherwise analytic. G_2 appears to have poles both at the poles of the functions Γ_2 and K_2 and at the zeros of the denominator which arise in the solution of Eq. (44). These latter poles are located at the solutions of

$$\det\left[\delta(ij)-\frac{J}{(2S)^2}K_2(i;j;\mathbf{K},z)\right]=0, \tag{45}$$

where $\delta(ij)$ and $K_2(i;j;\mathbf{K},z)$ are regarded as $d\times d$ matrices in the spatial directions i, $j=1,\cdots,d$. A care-

[8] When L is even and $K_i=\pi$, it is direct to compute $G_2(r;r';\mathbf{K},\omega)$ and to carry through the program outlined. There are a total of $[\frac{1}{2}N+1-\delta(2S-1)]$ states of $K_i=\pi$. All but d of these are degenerate at the energy $(2\mu+4SJd)$ of two independent spin waves of total momentum $(k_1)_i+(k_2)_i=\pi$. The remaining d states are shifted down in energy by the interaction to $(2\mu+J(4Sd-1))$ and have wave functions in which the two spin deviations are restricted to nearest neighbor sites. These states correspond to the bound states of Sec. 4.

ful analysis shows that the residue of G_2 at many of the apparent poles vanishes. A more detailed discussion of the poles of G_2 is contained in Appendix A. There is a close parallel in the treatment of two-particle scattering by a potential which can be expressed as a finite sum of factorizable potentials.[9] For our present purposes it is sufficient to point out that any pole of G_2 at the energy of two free spin waves is certainly not related to a bound state, so that the only poles of G_2 which can correspond to bound states are located at the roots of (45). The structure of (45) is analyzed in Appendix B. It is shown there that for given $\mathbf{K}$ most of the real solutions are interspersed between the poles, $[2\mu+S(\mathbf{k},\mathbf{K})]$, of Γ_2 and K_2 but that a small number of solutions may lie well outside these bounds. It is these solutions, shifted by the interaction outside the range of energies accessible to two free spin waves, which we shall identify with the bound states.

When N becomes large ($N\rightarrow\infty$), things are particularly clear, and it is only for this case that the concept of a bound state becomes entirely meaningful. As $N\rightarrow\infty$, the summations in (39) and (40) may for certain purposes[10] be replaced by integrations,

$$\frac{1}{N}\sum_{\mathbf{k}\epsilon\overline{F}}\rightarrow\frac{1}{(2\pi)^d}\int_{-\pi}^{\pi}(dk), \tag{46}$$

where (dk) represents a d-dimensional volume element. The functions $\Gamma_2(z)$ and $K_2(z)$ in this approximation have a cut along the real z axis,

$$[2\mu+S(\mathbf{0},\mathbf{K}),\ 2\mu+S(\pi,\mathbf{K})], \tag{47}$$

and are otherwise analytic. $G_2(z)$ may have in addition to the cut (47) discrete poles at the solutions of (45) lying outside the cut.[11] These solutions give the energies of the bound states of two interacting spin waves of total momentum $\mathbf{K}$. In Sec. 4 we turn our attention to the evaluation of the bound-state condition (45).

4. THE BOUND STATES OF TWO SPIN WAVES IN A LARGE LATTICE

The bound state condition (45) may be rewritten as

$$\det[2S\delta(ij)-B_2(ij)]=0, \tag{48}$$

where $\mathbf{K}$ and z have been left implicit and

$$B_2(ij)=\frac{1}{\pi^d}\int_0^{\pi}(dk)\frac{\cos k_i(\cos k_j-\alpha_j)}{t-\sum_l\alpha_l\cos k_l}, \tag{49}$$

with

$$t=d-\left(\frac{z-2\mu}{4SJ}\right)\quad\text{and}\quad 0\leqq\alpha_l=\cos\tfrac{1}{2}K_l\leqq 1. \tag{50}$$

As a function of the variable t, B_2 has a cut along the real axis $-\sum_l\alpha_l\leqq t\leqq\sum_l\alpha_l$. Possible bound states lie on the real t axis for $t\geqq|\sum_l\alpha_l|$. If $t_B(\mathbf{K})$ is a solution of (48) in this region for given $\mathbf{K}$, then

$$E_0+2\mu+4SJ[d-t_B(\mathbf{K})] \tag{51}$$

is the energy of a two-particle bound state of the Hamiltonian (6). Note that the condition (48) no longer depends on the exchange constant J except through t. For $\mu>0$, $J>0$ (ferromagnetic case) E_0 is the ground-state energy of the Heisenberg model, so $t_B\leqq d$. Our program, therefore, is to evaluate as far as possible the integrals (49) for $t\leqq-\sum_l\alpha_l$ and $\sum_l\alpha_l\leqq t\leqq d$, to look for solutions, t_B, of the bound-state condition (48), and to use (51) to compute the corresponding energy eigenvalues. Before examining separately the various dimensionalities, $d=1$, 2, 3, it is convenient to make some general remarks concerning the condition (48) and the integrals (49).

The rather cumbersome determinental condition (48) simplifies when all α_i's are equal, $\alpha_i=\alpha$, $i=1,\cdots,d$. Under these conditions $B_2(ii)=B_2(11)$, $B_2(ij)=B_2(12)$ for $i\neq j$, and (48) takes the form

$$[2S-B_2(11)-(d-1)B_2(12)]\times[2S-B_2(11)+B_2(12)]^{(d-1)}=0. \tag{52}$$

For general values of the α_i's it is convenient to define a set of integrals, D:

$$\begin{aligned}D_0(t)&=\frac{1}{\pi^d}\int_0^{\pi}\frac{(dk)}{t-\sum_l\alpha_l\cos k_l},\\ D_i(t)&=\frac{1}{\pi^d}\int_0^{\pi}(dk)\frac{\cos k_i}{t-\sum_l\alpha_l\cos k_l},\\ D_{ij}(t)&=D_{ji}(t)=\frac{1}{\pi^d}\int_0^{\pi}(dk)\frac{\cos k_i\cos k_j}{t-\sum_l\alpha_l\cos k_l}.\end{aligned} \tag{53}$$

The function $B_2(ij)$ is now expressed as

$$B_2(ij)=D_{ij}(t)-D_i(t)\alpha_j. \tag{54}$$

The integrals (53) satisfy a set of sum rules,

$$\begin{aligned}1&=tD_0(t)-\textstyle\sum_l D_l(t)\alpha_l,\\ tD_i(t)&=\textstyle\sum_j D_{ij}(t)\alpha_j,\end{aligned} \tag{55}$$

and have simple symmetry when the sign of t is reversed,

$$\begin{aligned}D_0(t)&=-D_0(-t),\\ D_i(t)&=D_i(-t),\\ D_{ij}(t)&=-D_{ij}(-t).\end{aligned} \tag{56}$$

For $d=1$, 2 the integrals D can be evaluated in terms of tabulated functions. Appendix C gives a representation of the D's as Laplace transforms of certain products of Bessel functions.

[9] M. Baker, Ann. Phys. (N.Y.) 4, 271 (1958).

[10] The replacement (46) misrepresents the summands of (39) and (40) over distances of order the reciprocal lattice spacing and will lead, therefore, to errors in energy shifts of order $1/N$ or in spatial wave functions over distances of order L.

[11] It is mathematically conceivable for the residue of the full G_2 to vanish at a zero of (45). Such a zero does not correspond to a two-particle energy eigenvalue. While this possibility cannot be excluded without more explicit calculation, it seems unlikely.

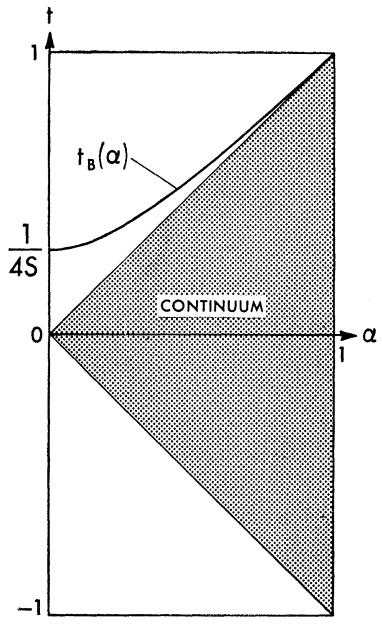

FIG. 1. Sketch of $t_B(\alpha)$ for the one-dimensional lattice. Equation (51) gives the relation between t_B and the energy of the bound states of two spin waves. $\alpha=\cos\frac{1}{2}K$.

Finally, when t is in the bound-state region, the D's and therefore the B_2's may be written as power series in (α_i/t),

$$B_2(ij)=\frac{1}{2t}+\frac{1}{t^3}\left(\frac{\alpha_i^2}{8}+\tfrac{1}{4}\sum_{l=1}^{d}\alpha_l^2\right)-\frac{\alpha_i^2}{2t^2}+O((\alpha/t)^4)$$
$$+O\left(\frac{1}{t}(\alpha/t)^4\right),\quad i=j \qquad (57)$$
$$=\alpha_i\alpha_j\left(\frac{1}{2t^3}-\frac{1}{2t^2}\right)+O((\alpha/t)^4)+O\left(\frac{1}{t}(\alpha/t)^4\right),$$
$$i\neq j.$$

It follows that for α_i small the solutions of (48) have the form

$$t_B(\mathbf{K})=(1/4S)+O(\alpha_i^2), \qquad (58)$$

i.e., for $K_i=\pi$ there are d bound states at the energy $E=E_0+2\mu+J(4Sd-1)$, in agreement with our previous result.[8] As the K_i become different from π, deviations of the bound state energy go as α_i^2. Note that when the α_i are near zero there are no bound states with negative t_B, i.e., above the energy cut for $J>0$.

Let us now examine the two-particle bound states in detail in one, two, and three dimensions.

A. The Bound States in One Dimension

Here an elementary integral gives

$$D_0(t)=\pm\frac{1}{(t^2-\alpha^2)^{1/2}}\quad\text{for}\quad t>\alpha\quad\text{or}\quad t<-\alpha. \qquad (59)$$

The bound-state condition (48) has the form,

$$2S\alpha^2(t^2-\alpha^2)^{1/2}=(t-\alpha^2)[t\mp(t^2-\alpha^2)^{1/2}]. \qquad (60)$$

For $t<-\alpha$ (lower sign) the signs of the two sides differ, so (60) can never be satisfied and there are no bound states. When $S=\frac{1}{2}$ the situation is particularly simple: Equation (60) yields immediately the unique solution,

$$t_B(K)=\tfrac{1}{2}(1+\alpha^2)\quad\text{or}\quad E=E_0+2\mu+\tfrac{1}{2}J(1-\cos K), \qquad (61)$$

which is precisely the energy of the bound spin complex found by Bethe.[2] For higher spin magnitudes and $t>\alpha$, it is convenient to rearrange (60) as

$$C(t)\equiv 4St^2[t+\alpha^2(S-1)]$$
$$=[t+(2S-1)\alpha^2]^2\equiv Q(t). \qquad (62)$$

The form of (62) guarantees that there is a unique solution, t_B, with $t>0$ for arbitrary K. The elementary inequalities, $C(\alpha)\leqq Q(\alpha)$ and $C(1)\geqq Q(1)$, show that $\alpha\leqq t_B\leqq 1$, as expected. For small α, t_B has the form

$$t_B(K)=(1/4S)+(3S-1)\alpha^2+O(\alpha^4). \qquad (63)$$

It is easy to show that $dt_B/d\alpha=1$ at $\alpha=1$. Note that the qualitative features of the curve $t_B(\alpha)$ are independent of S. Figure 1 summarizes these results. The energies of the continuum correspond to $-\alpha\leqq t\leqq\alpha$, so that the distance by which the curve $t_B(\alpha)$ lies above the curve $t=\alpha$ is, except for a factor of $4SJ$, just the binding energy of the bound spin pair at the corresponding total momentum, K.

B. The Bound States in Two Dimensions

Evaluation of the integrals D for the two-dimensional lattice is sketched in Appendix D. For $t\geqq\alpha_1+\alpha_2$ the results are

$$D_0(t)=kK(k)/\pi(\alpha_1\alpha_2)^{1/2},$$
$$D_i(t)=\frac{k}{\alpha_i\pi(\alpha_1\alpha_2)^{1/2}}[(t+\alpha_j)K(k)$$
$$-(t+\alpha_1+\alpha_2)\Pi(\beta_i^2,k)], \qquad (64)$$
$$D_{12}(t)=\frac{1}{k\pi(\alpha_1\alpha_2)^{1/2}}[(2-k^2)K(k)-2E(k)],$$

where

$$0\leqq k^2=\frac{4\alpha_1\alpha_2}{t^2-(\alpha_1-\alpha_2)^2}\leqq 1,\quad k\geqq 0,$$
$$\beta_i^2=\frac{-2\alpha_i}{t-\alpha_i+\alpha_j}\leqq 0,\quad \beta_1^2\beta_2^2=k^2,$$

and $i,j=1,2$ with $i\neq j$. The functions K, E, Π are, respectively, complete elliptic integrals of the first, second, and third kinds.[12] Equations (56) give the integrals D

[12] Paul F. Byrd and Morris D. Friedman, in *Handbook of Elliptic Integrals for Engineers and Physicists* (Springer-Verlag, Berlin, 1954), Eqs. 110.06–110.08.

when $t \leqq -\alpha_1-\alpha_2$. $D_{ii}(t)$ may be computed from (64) by use of the sum rule (55). For general α_i the complication of the bound-state condition (48) and the integrals (64) makes it difficult even to estimate t_B without resorting to numerical computation; however, certain special cases can be treated quite easily. These give a fairly clear idea of the behavior of the two-dimensional bound states.

If $\alpha_1=\alpha_2$, then $\beta_i^2=-k$, and II can be expressed in terms of the elliptical integral K.[13] The bound-state condition factors according to (52), giving

$$2S(2\alpha^2)/(t-2\alpha^2)=[(2/\pi)K(k)-1], \quad (65a)$$

$$2S(2\alpha^2)/t=[(4/\pi)E(k)-(1-k^2)(2/\pi)K(k)-1], \quad (65b)$$

where

$$1 \geqq k=2\alpha/|t| \geqq 0 \quad \text{and} \quad t^2 \geqq 4\alpha^2.$$

The right-hand side of (65a) and (65b) are always positive, while the left-hand side is negative for $t<0$, so there are no bound states with $t_B<0$, i.e., above the continuum for $J>0$. Equation (65a) has a unique solution for all $\alpha \neq 1$ with $2\alpha \leqq t_B \leqq 2$. If the ansatz, $t=2\alpha(1+\epsilon)$, $0<\epsilon \ll 1$, and the expansion[14]

$$K(k)=\ln(4/k')+O(k'^2 \ln k'),$$

$k'^2=1-k^2$ (valid when k' is small) are substituted into (65a), we obtain

$$\epsilon=8\exp\left(-\frac{2\pi S\alpha}{1+\epsilon-\alpha}\right). \quad (66)$$

Equation (66) has a solution for arbitrarily small α. If we adopt as a criterion of smallness $\epsilon \lesssim 1/100$, then the final formula for t_B,

$$t_B(\alpha) \cong 2\alpha\left[1+8\exp\left(-\frac{2\pi S\alpha}{1-\alpha}\right)\right], \quad (67)$$

is a very good approximation for $\alpha \gtrsim 7/(2\pi S+7)$. This result explicitly contradicts Dyson's[15] conclusion that there are no bound states in two dimensions. By contrast with (65a), Eq. (65b) does not have solutions for α near unity. Since both (65a) and (65b) have a single solution of the form (58) for small α, it is of interest to ask—for what value of α does (65b) develop a solution? It is reasonable to assert on the basis of physical continuity and the discussion of Appendix B

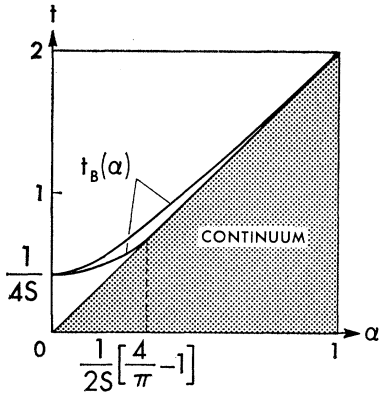

FIG. 2. Sketch of $t_B(\alpha)$ for the two-dimensional case $\alpha_1=\alpha_2=\alpha$. The lower branch merges with the continuum at $\alpha=(1/2S)\times[(4/\pi)-1]$. There are no bound states at negative t.

that at this threshold the corresponding curve $t_B(\alpha)$ merges with the continuum. Equation (65b) with $t=2\alpha$ yields directly the evaluation

$$0 \leqq \alpha=\frac{1}{2S}\left(\frac{4}{\pi}-1\right) \leqq 1 \quad (68)$$

for the threshold value of α. The bound-state curves, $t_B(\alpha)$, are sketched in Fig. 2.

The discussion in the last paragraph was limited to the symmetric case $\alpha_1=\alpha_2$. Solution is also possible in certain limiting cases for $\alpha_1 \neq \alpha_2$. When α_i is small, the expansion (57) gives

$$t_B=\frac{1}{4S}+\left(\frac{5S-1}{2}\right)(\alpha_1^2+\alpha_2^2) \pm \tfrac{1}{2}[(S-1)^2(\alpha_1^2+\alpha_2^2)^2 + 12S(5S-1)\alpha_1^2\alpha_2^2]^{1/2}+O(\alpha_i^4). \quad (69)$$

The ansatz $t=(\alpha_1+\alpha_2)(1+\epsilon)$, $0<\epsilon \ll 1$, makes the argument k of the various elliptic integrals appearing in the D's near one. Then the standard expansions[13,16] in $k'^2=1-k^2$ allow derivation of a self-consistent equation for ϵ similar to (66) but with a rather complicated argument for the exponential. This equation has a solution for α_i arbitrarily close to 1. The analog to (67) for $\alpha_1 \neq \alpha_2$ is rather messy; however, for $\alpha_i \approx 1$ it assumes the simple form

$$t_B(\alpha_1,\alpha_2) \cong (\alpha_1+\alpha_2)\left[1+8\exp\left(-\frac{(2\pi)(2S)}{2-\alpha_1-\alpha_2}\right)\right], \quad (70)$$

which reduces to (67) in the appropriate limit.

Finally, when $\alpha_2=0$, it follows that $D_2(t)=D_{12}(t)=0$ and $D_{22}(t)=\frac{1}{2}D_0(t)$, so the bound-state condition (48) factors:

$$[2S-B_2(11)][2S-\tfrac{1}{2}D_0(t)]=0. \quad (71)$$

The first factor gives a bound state of precisely the one-dimensional form, (61); the second leads to

$$t_B(\alpha_1,0)=+[(4S)^{-2}+\alpha^2{}_1]^{1/2}. \quad (72)$$

[13] P. F. Byrd and M. D. Friedman, in Ref. 12, Eq. 410.01.

[14] Herbert B. Dwight, *Tables of Integrals and Other Mathematical Data* (The MacMillan Company, New York, 1957), Eq. 773.3.

[15] F. J. Dyson, Phys. Rev. **102**, 1217 (1956), after Eq. (100). The origin of this discrepancy is not hard to find. Dyson's Eq. (100) is the correct bound-state condition for $\mathbf{K}=0$, i.e., $\alpha_i=1$, for which the only possible t_B is 2. For these values of α_i and t_B the bound-state condition does, indeed, fail. The point is that the bound-state integrals $B_2(ij)$ are highly singular as functions of α_i at $\alpha_i=1$. In particular it is clear from (49) that for $t=\alpha_1+\alpha_2$ the $B_2(ij)$ are finite if $\alpha_1=\alpha_2=1$ but logarithmically divergent for all other values of α_i.

[16] H. B. Dwight, Ref. 14, Eqs. 773.3 and 774.3.

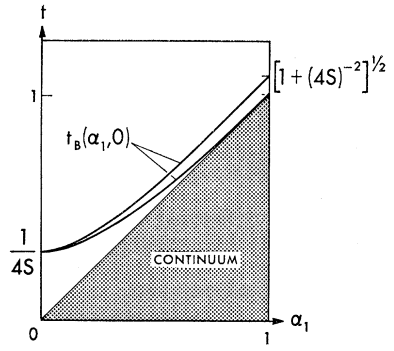

FIG. 3. Sketch of $t_B(\alpha_1,0)$ for the two-dimensional lattice. There are two bound states for each value of α_1.

Figure 3 depicts these results. There are no bound states for $t<0$. The situation is, of course, entirely similar when $\alpha_1=0\neq\alpha_2$.

When α_1 and α_2 are near zero, there are two bound states; when α_1 and α_2 are near unity, there is one. Without examining the bound-state condition (48) for arbitrary α_1 and α_2, it is impossible to conclude with complete rigor that there are always either one or two bound states; however, on the basis of the special cases which can be simply solved, it seems reasonable to conjecture that this is so. It then becomes of interest to plot in the α_1, α_2 plane the threshold for the appearance of the second bound state. The assumption [cf., the derivation of (68)] that the second bound state merges with the continuum at threshold associates the argument $k=1$ with the integrals (64) at threshold. As $k\rightarrow 1$, the functions $K(k)$ and $\Pi(\beta_i^2,k)$ are singular[16] as $\ln(1-k^2)$. When (48) is multiplied out, the terms quadratic in the singularity cancel. The condition for a bound state at the edge of the continuum is, therefore, that the coefficient of the remaining logarithmic singularity should vanish. This leads to the equation

$$\left[\pi S-\frac{\tau}{\alpha_1}+\frac{\gamma_1}{\alpha_1^2}(\alpha_1+\alpha_2-\alpha_1^2)+\gamma_2\frac{\alpha_1}{\alpha_2}\right](1-\alpha_2)$$
$$+\left[\pi S-\frac{\tau}{\alpha_2}+\frac{\gamma_2}{\alpha_2^2}(\alpha_1+\alpha_2-\alpha_2^2)+\gamma_1\frac{\alpha_2}{\alpha_1}\right](1-\alpha_1)=0, \quad (73)$$

where

$$\tau=(\alpha_1/\alpha_2)^{1/2}+(\alpha_2/\alpha_1)^{1/2}$$

and

$$\gamma_i=\sin^{-1}(\alpha_i/(\alpha_1+\alpha_2))^{1/2}.$$

The solutions of (73) include the threshold points already shown in Figs. 2 and 3. Near $\alpha_1=1$, $\alpha_2=0$ the curve (73) has the form

$$\alpha_2=(4/3\pi S)^2(1-\alpha_1)^2. \quad (74)$$

Figure 4 shows the threshold curve for the two-dimensional bound states.

In the special cases treated exactly there have been no bound states with $t<0$. Probably such bound states do not exist; however, a more careful discussion of (48) for arbitrary α_i would be necessary to decide this point with certainty.

C. The Bound States in Three Dimensions

The integrals D appropriate to the three-dimensional lattice are not to the author's knowledge available in analytic form for arbitrary values of the parameters t and α_i. Evaluations have, however, been carried out for certain special values of the parameters,[17] and these will suffice for us to form a good qualitative picture of the number and behavior of the bound states.

When $\alpha_i=\alpha$, the integrals D of (53) all have the simple property

$$D(t,\alpha)=(1/\alpha)D(t/\alpha,1). \quad (75)$$

Equations (52), (54), and (55) then give the bound-state conditions,

$$\tfrac{2}{3}S\alpha=(t/3\alpha)D_1(t/\alpha,1)-D_{12}(t/\alpha,1), \quad (76a)$$
$$\tfrac{2}{3}S\alpha=(t/3\alpha-\alpha)D_1(t/\alpha,1). \quad (76b)$$

The condition (76a) appears as a quadratic factor in (52), so its solutions are related to doubly degenerate bound states. Condition (76b) is nondegenerate. It is easy to show that for $t\geqq 3\alpha$, $D_1(t/\alpha,1)>0$. Dyson[17] uses an ingenious electric circuit analog to demonstrate further that $0<D_1(t/\alpha,1)-D_{12}(t/\alpha,1)<\frac{1}{12}$. These inequalities and use of (56) prove that bound states do not exist for $t\leqq -3\alpha$. According to the discussion after (51), bound states with $t>0$ must lie in $3\geqq t\geqq 3\alpha$. In particular, as $\alpha\rightarrow 1$, only $t\rightarrow 3$ is possible. The condition (76b) is obviously not satisfied for $\alpha=1$. Dyson's inequality shows that (76a) also fails. Therefore, there do not exist bound states of two spin waves with $\mathbf{K}=0$ in three dimensions. The integrals D defined by (53) are in three dimensions perfectly continuous functions of their variables, t and α_i, for $t\geqq\sum_l\alpha_l$. It follows that there exists a finite region around $\mathbf{K}=0$ ($\alpha_i=1$) for

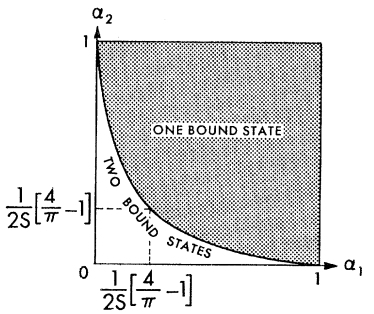

FIG. 4. Sketch of threshold for the appearance of the second bound state for each $\mathbf{K}$ for the two-dimensional lattice $\alpha_i=\cos\frac{1}{2}K_i$.

[17] G. N. Watson, Quart. J. Math. **10**, 266 (1939), computes D_0 for $\alpha_i=1=\frac{1}{3}t$. F. J. Dyson, Ref. 15, Eq. (89) and after Eq. (100), obtains useful inequalities for $\alpha_i=1$, $t\geqq 3$. J. G. Hanus, in *Quarterly Progress Report*, Solid State and Molecular Theory Group (MIT), **43**, 96 (1962), tabulates the equal α_i case for selected values of t and gives further references. He works from the Laplace transform representation (see Appendix C).

which there are no bound states.[18] Dyson[4] recognized this but went on to conjecture incorrectly that there were no bound states for arbitrary **K**. Equation (58) and footnote 8 already show that such bound states do exist for small α_i. The threshold for their appearance is easy to compute when $\alpha_i=\alpha$. As in two dimensions the bound states are expected to merge with the continuum at threshold, so we look for solutions of (76) with $t=3\alpha$:

$$\tfrac{2}{3}S\alpha=D_1(3,1)-D_{12}(3,1)=0.0618\,, \qquad (77a)$$

$$\tfrac{2}{3}S\alpha(1-\alpha)=D_1(3,1)=0.1721\,, \qquad (77b)$$

where Hanus'[17] values have been used for the integrals. It is direct to compute threshold values of α from Eqs. (77). For $S=\frac{1}{2}$ the thresholds correspond to $K_i=159°$ (doubly degenerate) and $K_i=140°$ (nondegenerate). These values agreed with those obtained by Hanus[19] in an analysis somewhat less direct than ours and

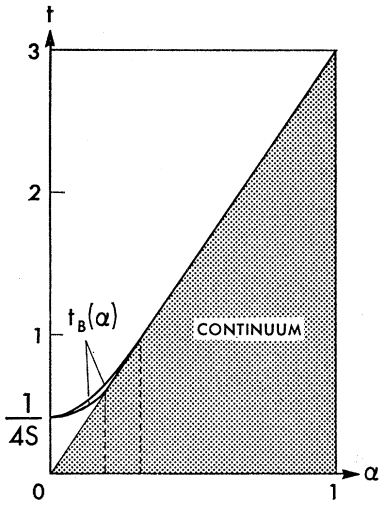

FIG. 5. Sketch of $t_B(\alpha)$ for the three-dimensional lattice and $\alpha_i=\alpha$. The lower curve is doubly degenerate. Threshold values of α are given by (77).

restricted to $S=\frac{1}{2}$, $d=3$. Figure 5 shows the bound-state behavior for $\alpha_i=\alpha$.

The three-dimensional analog of (69) for small α_i follows from (57). The resulting cubic equation has three solutions of the form (58). There are no solutions with $t<0$.

Finally, when one of the α_i's vanishes (i.e., on one of the faces of the **K** cube), the bound-state condition (48) factors in analogy to (71) into a two-dimensional and a one-dimensional part. If, for example, $\alpha_3=0$, the two-dimensional part gives just the bound states of Sec. 3B. In addition to these there are bound states at the solutions of $4S=D_0(t)$, with $D_0(t)$ given by (64).

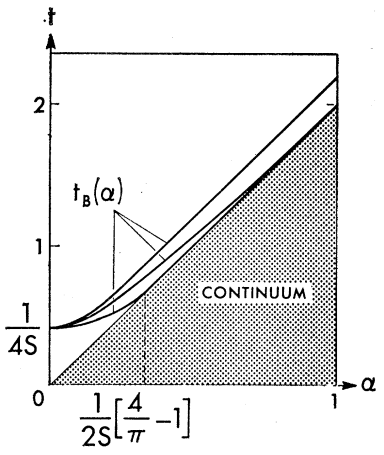

FIG. 6. Three-dimensional bound-state behavior for $\alpha_1=\alpha_2=\alpha$ and $\alpha_3=0$.

It is easy to verify that this condition leads always to a unique bound state with $t>\alpha_1+\alpha_2$. In particular for $\alpha_1=\alpha_2=1$, the corresponding t_B solves $4S\pi=(2/t)K(2/t)$, so $t_B>2$. In Fig. 6 the situation is pictured for $\alpha_1=\alpha_2=\alpha$, $\alpha_3=0$.

Complete solution of the three-dimensional bound-state problem depends on evaluation of the integrals D for arbitrary α_i. The special cases considered above do, however, provide a solid basis for speculation concerning the qualitative features of the full solution. There appear to be no bound states with $t<0$.[20] The α cube, $0\leqq\alpha_i\leqq1$, seems to be divided into four regions, according as there are 0, 1, 2, or 3 bound states with $t>0$ for each corresponding value of the total mo-

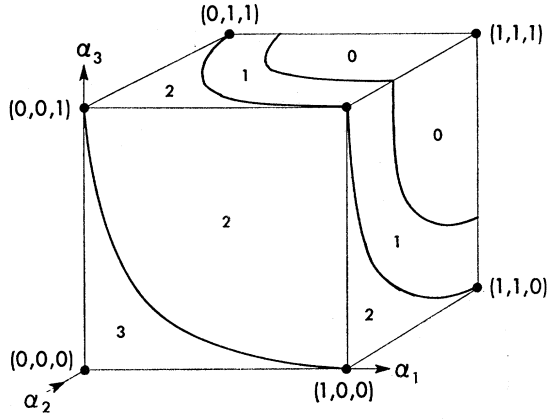

FIG. 7. Threshold surfaces in three dimensions, as they intersect the faces of the α cube. Numerals on the cube faces indicate the number of bound states for each set of $(\alpha_1,\alpha_2,\alpha_3)$ in the corresponding regions.

[18] Note that the singularity of the integrals D in two dimensions as $t\to\alpha_1+\alpha_2$ makes this argument inapplicable. See footnote 15.

[19] J. G. Hanus, in *Quarterly Progress Report*, Solid State and Molecular Theory Group (MIT), **43**, 96 (1962); **44**, 38 (1962); and **46**, 137 (1962). Hanus works from a Schrödinger equation and introduces a Green's function similar to our G_2 only as an auxiliary. The first paper treats the spin-wave interaction incorrectly. This error is rectified in the second.

[20] Hanus (Ref. 19) in his first paper claims to find bound states symmetrically above and below the continuum. He bases his argument on the "invariance of the trace of the interaction." It is hard to see how such an argument can (as his seems to) be independent of the phase shifts in the continuum. The present author believes that he has simply misrepresented the reflection properties (56) of the integrals D. In any case our calculations do not corroborate his conclusion.

mentum of the bound pair. Figure 7 shows a sketch of the intersections of the threshold surfaces defining these regions with the faces of the α cube and is the three-dimensional analog of Fig. 4. The analysis leading to Fig. 5 suggests that the two surfaces closest to $\alpha_1=\alpha_2=\alpha_3=0$ are tangent at the diagonal point $\alpha_1=\alpha_2=\alpha_3=(1/2S)(0.1854)$.

5. CONCLUSIONS

For a large, isotropic, d-dimensional, cubic Heisenberg model there may exist 0, 1, $\cdots$, d bound states of two spin waves, where the precise number depends in a complicated way on the total momentum of the bound pair. When J and μ are positive, so the states with small numbers of spin waves may be expected to be thermodynamically important at low temperatures, the bound states have energies below the two-particle continuum. Larger values of the total momentum favor larger numbers of bound states and larger binding energies relative to the continuum.[21] In particular for $d=3$, there are no bound states for total momenta that are sufficiently small. Even in two dimensions, where there are bound states for arbitrarily small $\mathbf{K}$, the corresponding binding energies go to zero exponentially with $\mathbf{K}$ [see Eq. (67)]. The qualitative features of the bound-state behavior are independent of the magnitude, S, of the individual spins.

Experimental observation of the bound states of two spin waves in materials well described by an isotropic Heisenberg model does not appear easy. Let us confine our remarks to the three-dimensional case with J, $\mu>0$, although experiments on thin films and chains are also conceivable. The present calculations have treated two spin waves in an otherwise aligned lattice. It is plausible to hope that at sufficiently low spin-wave densities, i.e., at sufficiently low temperatures, the spin waves will continue to exhibit predominantly single-particle and pair characteristics, so our treatment will remain accurate.[22] Dynamical experiments such as spin-wave resonance[23] and inelastic ferromagnetic neutron scattering[24] typically couple to single spin waves. Thus, such a process as creation of a bound pair either is of second order, and therefore, weak or must proceed via a spin wave already in the continuum, which makes analysis difficult. Alternatively, direct measurement of the low-temperature thermodynamics is quite feasible; however, the absence of bound states with small $\mathbf{K}$ means that there are continuum states lower by a finite energy gap, δ, than the lowest bound state. The effect of the bound states on the thermodynamics is, therefore, exponentially small with $e^{-\beta\delta}$.

These difficulties may not be insurmountable, but the situation is much simpler if one studies materials with a highly anisotropic exchange coupling. Consider, instead of the isotropic Hamiltonian (6),

$$H=\mu\sum_1 S^z(1)-\tfrac{1}{2}\sum_{1,2}J(12)[S^z(1)S^z(2)+\sigma S^+(1)S^-(2)]. \quad (78)$$

The Hamiltonian (78) incorporates an anisotropy parameter, $\sigma\geqq 0$. Isotropy corresponds to $\sigma=1$. The following discussion may be motivated by the observation that when $\sigma=0$, the Heisenberg model reduces to the Ising model, for which the bound states are always below the (degenerate) continuum. Notice that for $1\geqq\sigma\geqq 0$ and J, $\mu>0$ the fully aligned state is still the ground state. All the machinations of Secs. 2 and 3 go through just as before, only with factors of σ inserted at appropriate places. In particular, it is direct to verify that $G_1(1;1')$ is still given by (29), if in place of (30)

$$\Omega(\mathbf{k})=2SJ\sum_{i=1}^{d}(1-\sigma\cos k_i), \quad (79)$$

is used as the single-particle spectrum. Similarly, the integral equation (34) for G_2 remains valid, if the definition (35) is changed to

$$K_2(12;\bar{1}\bar{2})=\Gamma_2(12;\bar{1}\bar{2})-\tfrac{1}{2}\sigma[\Gamma_2(12;\bar{1}\bar{1})+\Gamma_2(12;\bar{2}\bar{2})] \quad (80)$$

and the correct G_1 is used in the evaluation (33) of Γ_2. The net effect is that Eq. (44) still gives $G_2(\mathbf{r};\mathbf{r}';\mathbf{K},\omega)$, if the terms $\cos(\frac{1}{2}\mathbf{K}\cdot\mathbf{r}')$ and $\cos(\frac{1}{2}K_i)$ appearing in the definitions (39)–(41) are multiplied by σ. The whole discussion of the bound states in Sec. 4 can then be carried over by simply changing the definition of α_i from (50) to

$$\alpha_i=\sigma\cos(\tfrac{1}{2}K_i), \quad 0\leqq\alpha_i\leqq\sigma. \quad (81)$$

Each of Figs. 1–7 is still correct; however, physical values of α_i are no longer $0\leqq\alpha_i\leqq 1$ but are given by (81). In the Ising limit, $\sigma=0$, Eqs. (58) and (51) show that there are always d-bound states degenerate at the energy $E_0+2\mu+J(4Sd-1)$, which is a trivial direct consequence of the Ising Hamiltonian.

Notice from Fig. 1 that for $0\leqq\sigma<1$ the one-dimensional bound-state curve never touches the continuum. For $S=\frac{1}{2}$, (51) and (61) give the bound-state energies as

$$E=E_0+2\mu+2SJ[1-\sigma^2\cos^2(\tfrac{1}{2}K)], \quad (82)$$

[21] The dependence of the number and binding energy of the bound states on the total momentum is a result of the discrete nature of the lattice and the consequent lack of invariance of the problem under continuous translations.

[22] Note that even at low densities the possibility of important corrections due to bound triplets, etc., cannot be rigorously excluded without examination of the three-particle problem, and so on. At temperatures near or above the Curie point, where roughly half the spins in the system are flipped, it seems likely that many particle effects will predominate and that the present discussion is entirely inapplicable.

[23] See, for example, P. E. Tannenwald, J. Phys. Soc. Japan **17**, Suppl. B-I, 592 (1962) and R. Kimura and H. Nosé, *ibid.*, 604 (1962). These authors give further references.

[24] See, for example, R. N. Sinclair and B. N. Brockhouse, Phys. Rev. **120**, 1638 (1960).

which has been obtained by Orbach.[25] Figure 4 shows that in two dimensions when $0\leqq\sigma\leqq(1/2S)(4/\pi-1)$ there are two bound states for each value of the total momentum.

In three dimensions for the phsyically interesting case J, $\mu>0$ Eq. (77b) shows that for

$$0\leqq\sigma<0.5163/(2S+0.5163) \tag{83}$$

there will be a bound state of $\mathbf{K}=0$ with energy lower than any continuum energy. For such an anisotropy the bound states will play a predominant role in determining the low-temperature thermodynamics, while the effect of the continuum states will be exponentially small as $T\rightarrow 0$. Under the pairing assumption[22] the characteristics of the two-particle bound-state spectrum should then be readily observable experimentally.

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APPENDIX A: THE POLES OF G_2

Because Eq. (44) does not mix different total momenta, it will be convenient to suppress explicit reference to $\mathbf{K}$ in what follows. Formulas (39) and (40) show that $\Gamma_2(\mathbf{r};\mathbf{r}';z)$ and $K_2(\mathbf{r};\mathbf{r}';z)$ regarded as functions of z are analytic everywhere except for a finite set of simple poles located on the real axis at the distinct values assumed by $(2\mu+S(\mathbf{k},\mathbf{K}))$ as $\mathbf{k}$ runs over the N modified reciprocal lattice points (42) with $\mathbf{K}$ fixed. Denote these poles by $\omega_n{}^{(0)}$. If $\gamma_n(\mathbf{r};\mathbf{r}')$ and $k_n(\mathbf{r};\mathbf{r}')$ are the residues of $\Gamma_2(z)$ and $K_2(z)$, respectively, at $z=\omega_n{}^{(0)}$, then

$$\Gamma_2(\mathbf{r};\mathbf{r}';z)=\sum_n\frac{\gamma_n(\mathbf{r};\mathbf{r}')}{z-\omega_n{}^{(0)}}, \tag{A1}$$

$$K_2(\mathbf{r};\mathbf{r}';z)=\sum_n\frac{k_n(\mathbf{r};\mathbf{r}')}{z-\omega_n{}^{(0)}}. \tag{A2}$$

Equation (20) guarantees that a similar representation exists for the function $G_2(z)$

$$G_2(\mathbf{r};\mathbf{r}';z)=\sum_n\frac{g_n(\mathbf{r};\mathbf{r}')}{z-\omega_n}, \tag{A3}$$

where ω_n are the true two-particle energy eigenvalues, which do not, in general, coincide with the $\omega_n{}^{(0)}$, and $g_n(\mathbf{r};\mathbf{r}')$ are the corresponding residues. Assume that one of the true two-particle energies falls at an unperturbed energy, so $\omega_m=\omega_m{}^{(0)}$. If (A1)–(A3) are substituted in the right-hand side of (44), the second term appears to give a second-order pole in $G_2(\mathbf{r};\mathbf{r}';z)$ at $z=\omega_m{}^{(0)}$, which contradicts (A3). The condition that this contradiction should not occur is

$$\textstyle\sum_j k_m(\mathbf{r};j)g_m(j;\mathbf{r}')=0. \tag{A4}$$

Since (A4) must hold for arbitrary $\mathbf{r}$, it follows that either $g_m(j;\mathbf{r}')=0$ or every $d\times d$ submatrix of $k_m(\mathbf{r};j)$ is singular. Assume for the moment that $k_m(\mathbf{r};j)$ has at least one nonsingular $d\times d$ submatrix, so $g_m(j;\mathbf{r}')=0$. Then the value of $g_m(\mathbf{r};\mathbf{r}')$ can be constructed entirely from $k_m(\mathbf{r};j)$ and $\gamma_m(\mathbf{r};\mathbf{r}')$. To do this, notice that the part of (44) singular at $z=\omega_m{}^{(0)}$ reads,

$$g_m(\mathbf{r};\mathbf{r}')=\gamma_m(\mathbf{r};\mathbf{r}')h_2(\mathbf{r}')+\frac{J}{(2S)^2}\sum_i k_m(\mathbf{r},j)G_2(j;\mathbf{r}';\omega_m{}^{(0)}). \tag{A5}$$

When $\mathbf{r}\equiv i$, the left-hand side vanishes and (A5) can be inverted to give $G_2(j;\mathbf{r}';\omega_m{}^{(0)})$. The resulting expression reinserted in (A5) evaluates,

$$g_m(\mathbf{r};\mathbf{r}')=[\gamma_m(\mathbf{r};\mathbf{r}')-\textstyle\sum_{ij}k_m(\mathbf{r};i)k_m{}^{-1}(i;j)\gamma_m(j;\mathbf{r}')]h_2(\mathbf{r}'), \tag{A6}$$

where $k_m{}^{-1}(i;j)$ is the matrix inverse of the $d\times d$ matrix $k_m(i;j)$. We are now in a position to draw two conclusions: (i) If $k_m(\mathbf{r},j)$ has a nonsingular $d\times d$ submatrix and the right-hand side of (A6) vanishes, then $G_2(\mathbf{r};\mathbf{r}';z)$ certainly does not have a pole at $\omega_m{}^{(0)}$ and (ii) if $k_m(\mathbf{r};j)$ has a nonsingular $d\times d$ submatrix and the right-hand side of (A6) does not vanish or if $k_m(\mathbf{r};j)$ is entirely singular, then $G_2(\mathbf{r};\mathbf{r}';z)$ may have a pole at $\omega_m{}^{(0)}$. Examples will be given in what follows.

Consider the one-dimensional case. Here (41) shows that except for the special case[8] $K=\pi$ there is a unique unperturbed energy, $\omega_k{}^{(0)}$, for each value of the magnitude of k. Thus,

$$\gamma_k(r;r')=\frac{(-2)(2S)^2}{N}m\cos kr\cos kr' \tag{A7}$$

and

$$k_k(r;r')=\frac{(-2)(2S)^2}{N}m\cos kr(\cos kr'-\cos\tfrac{1}{2}Kr'), \tag{A8}$$

where the multiplicity, m, is two or one depending on whether the particular k in question does or does not have a reflection in the modified zone (42). So long as $2k\neq K$, it is easy to verify that the hypotheses of conclusion (i) are satisfied and $G_2(z)$ has no poles at $[2\mu+S(k,K)]$. When $2k=K$, every component of $k_k(r,i)$ vanishes, and (44) shows that $G_2(z)$ does indeed have a pole at $[2\mu+S(\frac{1}{2}K,K)]$. In the special case[8] L even, $K=\pi$, $\Gamma_2(z)$ and $K_2(z)$ each has a single pole at $(2\mu+4SJ)$. Expressions (A7) and (A8) no longer hold.

[25] R. Orbach, Phys. Rev. 112, 309 (1958).

One finds that γ_n and k_n are diagonal in the magnitudes $|r|$ and $|r'|$; therefore, the right-hand side of (A6) vanishes for $|r|\neq|r'|$ and for $|r|=|r'|=1$, the hypotheses of (i) apply, and the corresponding $G_2(z)$'s do not have poles at $(2\mu+4SJ)$. When $|r|=|r'|\neq 1$, the right-hand side of (A6) is nonvanishing, and $G_2(z)$ may by (ii) have a pole at $(2\mu+4SJ)$. Examination of (44) shows that this does happen.

The higher dimensionalities are more difficult to analyze, since (41) no longer allows assignment of a unique $\omega_n^{(0)}$ for each $|\mathbf{k}|$. This added possibility for degeneracy makes it hard to exhibit the residues, γ_n and k_n, explicitly. In any case, it is clear that as $N\rightarrow\infty$ any poles of $G_2(z)$ at $\omega_n^{(0)}$ cannot lie outside the continuum; therefore, only solutions of (45) can contribute bound states.

APPENDIX B: THE STRUCTURE OF EQUATION (45)

Consider first the one-dimensional problem, which will exhibit all of the qualitative features of the more general problem. The characteristics of the function $[|J|/(2S)^2]K_2(1;1;K;\omega)$ may be read off from (A2) and (A8). There are a set of simple poles at the values $\omega=\omega_k^{(0)}\equiv 2\mu+4SJ(1-\cos k\cos\frac{1}{2}K)$. The residue at the pole $\omega_k^{(0)}$ is positive when $0<\cos k<\cos\frac{1}{2}K$, zero when $\cos k=0$ or $\cos k=\cos\frac{1}{2}K$, and negative when $\cos k<0$ or $\cos k>\cos\frac{1}{2}K$. Figure 8 shows a typical sketch of $[J/(2S)^2]K(\omega)$, $J>0$, plotted as a function of the real variable ω. All but one of the solutions of (45) lie between the various poles, $\omega_k^{(0)}$. Only the leftmost branch of the curve contains a solution outside of these values. As $L\rightarrow\infty$ the solutions between the $\omega_k^{(0)}$ merge into a continuum; however, the left-most solution may (and does, in this case) remain separated from the continuum by a finite gap. This represents the effect of the two-particle interaction in splitting off a bound state from the continuum.

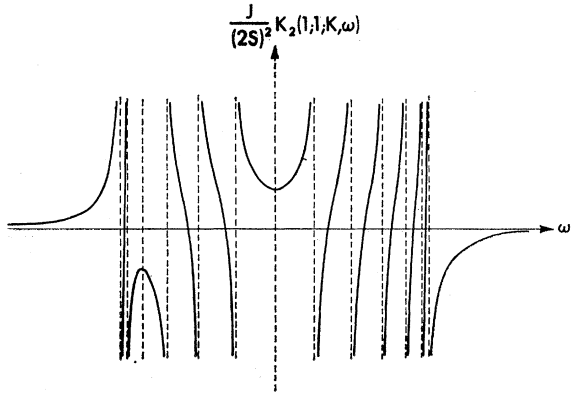

FIG. 8. Sketch of $[J/(2S)^2]K_2(1;1;K,\omega)$ for $J>0$. Numbers used are $L=24$, $LK/2\pi=2$. Dashed vertical lines indicate energies of two free spin waves. Depending on the location of unity on the vertical scale, the condition (45) may have one solution well below the continuum.

The extra matrix complexity of (45) for higher dimensionalities does not change the main conclusion: Most of the solutions of (45) lie between the unperturbed energies $\omega_n^{(0)}$ and, in the limit $N\rightarrow\infty$, merge into a continuum; however, a small number lie outside the range of values bounded by the $\omega_n^{(0)}$ and, as $N\rightarrow\infty$, may continue to exist as isolated poles of G_2 outside the continuum.

APPENDIX C: REPRESENTATION OF THE D FUNCTIONS

For values of t above the cut, $t\geqq\sum_l\alpha_l$, the representations

$$\frac{1}{t-\sum_l\alpha_l\cos k_l}=\int_0^\infty dp\,\exp[-(t-\textstyle\sum_l\alpha_l\cos k_l)p] \quad \text{(C1)}$$

and

$$I_n(p)=\frac{1}{\pi}\int_0^\pi d\alpha\, e^{p\cos\alpha}\cos n\alpha\,, \quad \text{(C2)}$$

where $I_n(p)$ is the Bessel function of imaginary argument of nth order,[26] allow the integrals (53) to be written,

$$D_0(t)=\int_0^\infty dp\, e^{-tp}\prod_l I_0(\alpha_l p)\,, \quad \text{(C3)}$$

$$D_i(t)=\int_0^\infty dp\, e^{-tp}I_1(\alpha_i p)\prod_{l\neq i} I_0(\alpha_l p)\,, \quad \text{(C4)}$$

$$D_{ii}(t)=\int_0^\infty dp\, e^{-tp}\tfrac{1}{2}[I_2(\alpha_i p)+I_0(\alpha_i p)]\prod_{l\neq i} I_0(\alpha_l p)\,, \quad \text{(C5)}$$

$$D_{ij}(t)=\int_0^\infty dp\, e^{-tp}I_1(\alpha_i p)I_1(\alpha_j p)\prod_{l\neq i,l\neq j} I_0(\alpha_l p)\,,\quad i\neq j\,. \quad \text{(C6)}$$

When t is below the cut, $t\leqq-\sum_l\alpha_l$, the reflection properties (56) determine the values of the D's.

APPENDIX D: EVALUATION OF THE D FUNCTIONS IN TWO DIMENSIONS

It is more than likely that the integrals (53) have been evaluated either directly or in the representation of Appendix C; however, the present author was unable to find such an evaluation except for special cases. He, therefore, feels that it may be useful to sketch a program by which these integrals may be reduced to more familiar forms.

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[26] H. B. Dwight, Ref. 14, Eq. 813.3, and Wilhelm Magnus and Fritz Oberhettinger, *Formulas and Theorems for the Functions of Mathematical Physics* (Chelsea Publishing Company, New York, 1954), p. 26.

Use the form (53) and assume $t \geqq \alpha_1+\alpha_2$. It is always easy to integrate over one component of $\mathbf{k}$, say k_2, by use of the formula,

$$\frac{1}{\pi}\int_0^\pi dk_2 \frac{\cos nk_2}{x-\cos k_2} = \frac{(x-(x^2-1)^{1/2})^n}{(x^2-1)^{1/2}}. \quad \text{(D1)}$$

Those of the resulting integrals which are not trivial may be transformed by the substitutions,

$$k_1=\pi-2\theta,$$
$$0 \leqq n_2^2 \equiv \frac{2\alpha_1}{t+\alpha_1+\alpha_2} \leqq \frac{2\alpha_1}{t+\alpha_1-\alpha_2} \equiv n_1^2 \leqq 1, \quad \text{(D2)}$$

into expressions of the type,

$$\frac{2}{\pi}\int_0^{\pi/2} d\theta \frac{(\sin\theta)^{2\nu}}{[(1-n_1^2\sin^2\theta)(1-n_2^2\sin^2\theta)]^{1/2}}, \quad \nu \text{ integral}, \quad \text{(D3)}$$

times certain factors involving the α_l. These integrals in turn yield to the elliptic substitution,[27]

$$\mathrm{sn}^2 u = \frac{(1-n_2^2)\sin^2\theta}{1-n_2^2\sin^2\theta}, \quad \text{(D4)}$$

giving the results (64).

[27] P. F. Byrd and M. D. Friedman, Ref. 12, Eqs. 284, 336, and 337.

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Magnetic-Field Dependence of Free-Carrier Absorption in Semiconductors*

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A plane-wave semiclassical analysis of the amplitude of an electromagnetic wave transmitted through a semiconductor in the presence of a magnetic field is discussed and some theoretical predictions are compared with experimental measurements. The Faraday and the Voigt configurations, longitudinal and transverse, respectively, are specifically considered. The theoretical results, obtained formally in terms of the high-frequency conductivity tensor, are applied to the isotropic, one-carrier semiconductor model. The general expression, covering all ranges of frequency and magnetic field within the extent of validity of the model, is derived and reduced to simple forms applicable to specific experimental situations. The problem is then generalized to ellipsoidal surfaces of constant energy, and to systems involving more than one type of carrier. Results of room temperature microwave experiments carried out in the Faraday configuration on silicon and germanium show, in general, good agreement with the theoretical analysis. Effects of magnetodichroism, observed in *n*-type silicon in this configuration, are reported. It is finally noted that the theoretical analysis of the Voigt configuration predicts the major features of the line shapes observed in far infrared experiments by other workers.

INTRODUCTION

MAGNETO-OPTICAL phenomena involving changes in the state of polarization of a wave, such as the Faraday or the Voigt effects, have recently received much attention as experimental tools for investigating transport properties of semiconductors. In this article, we analyze the magnetic-field dependence of the total absorption associated with the above phenomena, in the attempt to see what further information can be obtained by measuring transmitted amplitude as a function of the field. It will be shown that the effect provides a means of investigating the magnetic-field dependence of the diagonal component of the conductivity tensor, and represents in fact a modified high-frequency version of magnetoresistance. The changes in the amplitude of the transmitted wave can be quite pronounced in the free-carrier region and, in general, involve simple measuring techniques. It is thus worthwhile to consider the effect as a useful high-frequency method for the study of galvanomagnetic properties.

We will first outline a plane-wave semiclassical analysis of the case when an initially linearly polarized wave travels along the direction of an applied magnetic field. This situation gives rise to the Faraday effect, and will be referred to as the Faraday configuration. We will then consider the case of propagation transverse to the applied field, i.e., the Voigt configuration. Results of some microwave and infrared experiments carried out

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