Spin-Wave–Spin-Wave Scattering in a Heisenberg Ferromagnet*

R. G. BOYD† AND JOSEPH CALLAWAY
University of California, Riverside, California
(Received 21 January 1965)

We have obtained an exact solution describing the scattering of two spin waves in a simple cubic Heisenberg ferromagnet by solving the Lippmann-Schwinger equation for states with two spin deviations. The scattering amplitude is infinite at the energies of bound states discovered by Wortis, and the cross section agrees at long wavelengths with the approximate result obtained by Dyson. The methods used here are relatively conventional, and are generally applicable to any situation in which two excitations in a lattice interact via short-range forces.

INTRODUCTION

WE have obtained an exact solution describing the scattering of two spin waves in a simple Heisenberg ferromagnet by solving the Lippmann-Schwinger[1] equation (the integral form of the Schrödinger equation) for states with two spin deviations.

The scattering amplitude has poles at the energies of bound states discovered earlier by Wortis[2] and Hanus[3] through the solution of the equation of motion of the appropriate Green's function. The cross section agrees at long wavelengths with the approximate result of Dyson[4] for the ideal spin-wave system which he considered.

The methods we have used (discussed at greater length by one of us[5] in another paper) are more conventional than those used by Wortis or Dyson. They are generally applicable to any situation in which two excitations in a solid interact via short-range forces. A brief account of this work has been published previously.[6]

In this calculation we have neglected the Zeeman energy in an external magnetic field since it commutes with the Heisenberg exchange Hamiltonian and is hence a constant of motion. We have also neglected the magnetic dipole-dipole interaction, primarily because our methods are adapted to the treatment of short range forces only. We share this omission with Wortis, Dyson, and other authors who have treated the spin-wave–spin-wave interaction problem.[7]

Our unit of energy will be the Heisenberg exchange integral J. Our unit of distance will be the lattice parameter. We shall use the usual periodic boundary conditions on a cube containing N atoms with N very large.

* Research supported by U. S. Air Force Office of Scientific Research.
† National Science Foundation Predoctoral Fellow.

[1] B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950).
[2] M. Wortis, Phys. Rev. **132**, 85 (1963). See also N. Fukuda and M. Wortis, J. Phys. Chem. Solids **24**, 1675 (1963).
[3] J. Hanus, Phys. Rev. Letters **11**, 336 (1963).
[4] F. J. Dyson, Phys. Rev. **102**, 1217 (1956).
[5] J. Callaway, J. Math. Phys. **5**, 784 (1964).
[6] R. G. Boyd and J. Callaway, Phys. Rev. Letters **12**, 540 (1964).
[7] The scattering of spin waves through the dipole-dipole interaction is discussed by R. G. Boyd, Ph.D. thesis, University of California, Riverside, 1964 (unpublished).

SPIN OPERATOR FORMALISM IN A HEISENBERG FERROMAGNET

Consider a simple cubic lattice with a spin operator $\mathbf{S}_\mathbf{j}$ attached to each lattice site $\mathbf{j}$. The fundamental commutation relations for these operators are

$$\mathbf{S}_\mathbf{j}\times\mathbf{S}_\mathbf{j}=i\mathbf{S}_\mathbf{j},\quad [\mathbf{S}_\mathbf{i},\mathbf{S}_\mathbf{j}]_{\mathbf{i}\neq\mathbf{j}}=0. \tag{1}$$

We shall also have occasion to use the operators $S_\mathbf{j}^+$ and $S_\mathbf{j}^-$, defined in terms of vector components by the relations

$$S_\mathbf{j}^{\pm}=S_\mathbf{j}^x\pm iS_\mathbf{j}^y. \tag{2}$$

In terms of the latter operators the commutation relations become

$$[S_\mathbf{j}^+,S_\mathbf{k}^-]=2S_\mathbf{j}^z\delta_{\mathbf{jk}},\quad [S_\mathbf{j}^z,S_\mathbf{k}^\pm]=\pm S_\mathbf{k}^\pm\delta_{\mathbf{jk}}. \tag{3}$$

In the Heisenberg model of a ferromagnet the Hamiltonian is given by

$$H=-\sum_{\mathbf{j}\Delta}\mathbf{S}_\mathbf{j}\cdot\mathbf{S}_{\mathbf{j}+\Delta}, \tag{4}$$

where the index $\mathbf{j}+\boldsymbol{\Delta}$ indicates the nearest-neighbor lattice site connected to site $\mathbf{j}$ by the primitive lattice vector $\boldsymbol{\Delta}$. The Hamiltonian can be written in terms of components as

$$H=-\sum_{\mathbf{j}\Delta}\{S_\mathbf{j}^zS_{\mathbf{j}+\Delta}^z+S_\mathbf{j}^+S_{\mathbf{j}+\Delta}^-\}. \tag{5}$$

Define the total angular momentum

$$\mathbf{J}=\sum_\mathbf{j}\mathbf{S}_\mathbf{j}. \tag{6}$$

We find that

$$[H,\mathbf{J}]=0 \tag{7}$$

so that $\mathbf{J}^2$ and J^z are constants of motion.

We define a "number of spin deviations" operator by

$$n=NS+J^z \tag{8}$$

and proceed to discuss the subspaces invariant under H which are characterized by $n=0$, 1, 2.

SUBSPACE $n=0$

We denote by $|0\rangle$ (assumed normalized) the state of total alignment defined by

$$S_\mathbf{j}^-|0\rangle=0,\quad \text{every } \mathbf{j}. \tag{9}$$

It is an eigenfunction of H, J, n with eigenvalues of $-NZS^2$, NS, and 0, respectively. Z is the number of nearest neighbors; 6 in our case. Since the zero point of energy is of no fundamental significance, we shall reset it in each subpace to avoid repeating nonessential constants in our equations. Here, for instance, we add NZS^2 to H so that

$$H|0\rangle=0. \tag{10}$$

SUBSPACE $n=1$

We generate the vectors of this subspace from the previously defined ground state $|0\rangle$ by operating once with the ladder operators S_j^+. Define

$$|\mathbf{j}\rangle=S_j^+|0\rangle. \tag{11}$$

This is a single deviation state ($n=1$). To evaluate the effect of H operating on $|j\rangle$ we require the commutator

$$[H,S_j^+]=2\sum_{\Delta}\{S_{j+\Delta}^+S_j^z-S_j^+S_{j+\Delta}^z\}. \tag{12}$$

Since

$$H|\mathbf{j}\rangle=[H,S_j^+]|0\rangle+S_j^+H|0\rangle, \tag{13}$$

we have

$$H|\mathbf{j}\rangle=2S\sum_{\Delta}\{|\mathbf{j}\rangle-|\mathbf{j}+\mathbf{\Delta}\rangle\}. \tag{14}$$

As is well known, the Hamiltonian can be diagonalized by Fourier transformation. We define the spin-wave states $|\lambda\rangle$ in terms of the localized states $|j\rangle$ by

$$|\lambda\rangle=N^{-1/2}\sum_{\mathbf{j}}\exp(i\lambda\cdot\mathbf{j})|\mathbf{j}\rangle \tag{15}$$

with the inverse transformation

$$|\mathbf{j}\rangle=N^{-1/2}\sum_{\lambda}\exp(-i\lambda\cdot\mathbf{j})|\lambda\rangle. \tag{16}$$

Since

$$H|\lambda\rangle=2S(Z-\sum_{\Delta}\cos\lambda\cdot\mathbf{\Delta})|\lambda\rangle, \tag{17}$$

the spin-wave states $|\lambda\rangle$ are eigenstates of H with eigenvalue

$$E_\lambda=2S(Z-\sum_{\Delta}\cos\lambda\cdot\mathbf{\Delta}). \tag{18}$$

They are also eigenstates of J^2. The identity

$$[\mathbf{J}^2,S_j^+]=2(J^zS_j^+-J^+S_j^z)-ZS_j^+ \tag{19}$$

enables us to show that

$$J^2|\lambda\rangle=[NS(NS-1)+2NS\delta(\lambda)]\lambda\rangle. \tag{20}$$

We write occasionally $\delta(\lambda)$ for $\delta_{\lambda,0}$. The exceptional state $\lambda=0$ has $J=NS$, but its energy is continuous at $\lambda=0$ with the energy of the other states for which $J=NS-1$.

The norms of $|\lambda\rangle$ and $|j\rangle$ are given by

$$\langle\lambda|\lambda\rangle=\langle\mathbf{j}|\mathbf{j}\rangle=2S. \tag{21}$$

Distinct vectors in either set are orthogonal.

SUBSPACE $n=2$

We apply the ladder operators S_j^+ once to each of the vectors in the preceding subspace to generate the two deviation states

$$|\mathbf{jk}\rangle=S_j^+S_k^+|0\rangle. \tag{22}$$

Since $|\mathbf{jk}\rangle$ and $|\mathbf{kj}\rangle$ are the same state, our set of states is redundant if we let $\mathbf{j}$ and $\mathbf{k}$ run independently through all values. The norm of $|\mathbf{jk}\rangle$ is given by

$$\langle\mathbf{jk}|\mathbf{jk}\rangle=4S^2(1-\delta_{jk}/2S)(1+\delta_{jk}). \tag{23}$$

Hence, if $S=\frac{1}{2}$, the vectors $|\mathbf{jj}\rangle$ are null vectors and do not represent physical states at all. Finally, we note that distinct vectors of the set are orthogonal.

The effect of H operating on $|\mathbf{jk}\rangle$ is given by

$$H|\mathbf{jk}\rangle=S_j^+S_k^+H|0\rangle+S_j^+[H,S_k^+]|0\rangle+S_k^+[H,S_j^+]|0\rangle+[[H,S_j^+],S_k^+]|0\rangle. \tag{24}$$

The first term yields the ground-state energy (which we have set equal to zero). The second and third terms can be diagonalized on Fourier transformation, just as in the single deviation subspace, yielding the energies of two free spin waves as in Eq. (17). The fourth term evidently represents the interaction between the two spin waves, for the evaluation of which we require the commutator

$$[[H,S_j^+],S_k^+]=2\sum_{\Delta}\{\delta_{j,k}-\delta_{j+\Delta,k}\}S_j^+S_{j+\Delta}^+. \tag{25}$$

In accordance with these remarks, it is natural to define (for a basis) the set of two-spin-wave states

$$|\lambda\lambda'\rangle=N^{-1}\sum_{\mathbf{jj}'}\exp[i\lambda\cdot\mathbf{j}+i\lambda'\cdot\mathbf{j}']|\mathbf{jj}'\rangle \tag{26}$$

with the inverse transformation

$$|\mathbf{jj}'\rangle=N^{-1}\sum_{\lambda\lambda'}\exp[-i\lambda\cdot\mathbf{j}-i\lambda'\cdot\mathbf{j}']|\lambda\lambda'\rangle. \tag{27}$$

Equation (24) becomes

$$H|\lambda\lambda'\rangle=2S\sum_{\Delta}(2-\cos\lambda\cdot\mathbf{\Delta}-\cos\lambda'\cdot\mathbf{\Delta})|\lambda\lambda'\rangle+2N^{-1}\times\sum_{\mathbf{j}\Delta}(1-\cos\lambda'\cdot\mathbf{\Delta})\exp(i\lambda\cdot\mathbf{j}+i\lambda'\cdot\mathbf{j})|\mathbf{jj}+\mathbf{\Delta}\rangle, \tag{28}$$

where the interaction term may alternatively be written as

$$2N^{-1}\sum_{\mathbf{kk}'\Delta}\delta_{\lambda+\lambda',\mathbf{k}+\mathbf{k}'}(1-\cos\lambda'\cdot\mathbf{\Delta})\times\exp(-i\mathbf{k}'\cdot\mathbf{\Delta})|\mathbf{kk}'\rangle. \tag{29}$$

Unfortunately, the set of states defined in Eq. (26) has the scalar product

$$\langle\mathbf{kk}'|\lambda\lambda'\rangle=4S^2\delta_{\lambda+\lambda',\mathbf{k}+\mathbf{k}'}\{\delta_{\lambda\mathbf{k}}+\delta_{\lambda\mathbf{k}'}-1/NS\}. \tag{30}$$

so that the set is neither orthogonal nor normal. The set is also redundant since $|\lambda\lambda'\rangle$ and $|\lambda'\lambda\rangle$ are the same state.

Since the departure from orthogonality is small, we expect that we can achieve an orthonormal set with only minor changes in our formalism. First, however, we shall eliminate the total wave vector from the problem since it is preserved by the interaction, and since states of different total wave vector are orthogonal. We switch to new coordinates in momentum space, the total wave vector $\mathbf{K}$ and relative wave vector

$$\mathbf{K}=\boldsymbol{\lambda}+\boldsymbol{\lambda}', \quad \boldsymbol{\tau}=\tfrac{1}{2}(\boldsymbol{\lambda}-\boldsymbol{\lambda}'). \tag{31}$$

Also, since the norm of the state $|\mathbf{jj}'\rangle$ and the interaction between the two spin deviations depend only on the relative distance between the two deviations, we switch to the conjugate coordinates in position space, the center $\mathbf{C}$ and separation $\mathbf{R}$

$$\mathbf{C}=\tfrac{1}{2}(\mathbf{j}+\mathbf{j}'), \quad \mathbf{R}=\mathbf{j}-\mathbf{j}'. \tag{32}$$

We eliminate the coordinates $\boldsymbol{\lambda}$ in momentum space and $\mathbf{C}$ in position space by defining the mixed orthonormal basis

$$|\mathbf{KR}\rangle=N^{-1/2}\sum_{\mathbf{C}}\exp(i\mathbf{K}\cdot\mathbf{C}) \times[2S(2S-\delta_{\mathbf{R},0})(1+\delta_{\mathbf{R},0})]^{-1/2}|\mathbf{CR}\rangle \tag{33}$$

with orthonormality relations

$$\langle\mathbf{K}'\mathbf{R}'|\mathbf{KR}\rangle=\delta_{\mathbf{K},\mathbf{K}'}\{\delta_{\mathbf{R}',\mathbf{R}}+\delta_{\mathbf{R}',-\mathbf{R}}\}[1+\delta_{\mathbf{R},0}]^{-1}. \tag{34}$$

For $S=\frac{1}{2}$, there is no physical vector $|\mathbf{K}0\rangle$. However, for convenience in calculation we adjoin such a vector to our space.

In terms of this basis Eq. (24) becomes

$$H|\mathbf{R}\rangle=-2\delta_{\mathbf{R}\Delta}|\mathbf{R}\rangle-2\sum_{\Delta}\cos\tfrac{1}{2}(\mathbf{K}\cdot\boldsymbol{\Delta})\left[\frac{1+\delta_{\mathbf{R},-\Delta}}{1+\delta_{\mathbf{R},0}}\right]^{1/2} \times[(2S-\delta_{\mathbf{R},0})(2S-\delta_{\mathbf{R},-\Delta})]^{1/2}|\mathbf{R}+\boldsymbol{\Delta}\rangle. \tag{35}$$

We omit the total wave vector as an index since H is diagonal in $\mathbf{K}$. Also, we have subtracted $4SZ$ from H to eliminate a constant. Note that for $S=\frac{1}{2}$, there is no matrix element for H between the unphysical state $|\mathbf{K}0\rangle$ and the physical states, so that our use of the unphysical state cannot affect our solution for the amplitude on the physical states.

Now we define new two-spin-wave states in terms of the mixed orthonormal basis

$$|\mathbf{K}\boldsymbol{\tau}\rangle=N^{-1/2}\sum_{\mathbf{R}}\exp(i\boldsymbol{\tau}\cdot\mathbf{R})\left[\frac{1+\delta_{\mathbf{R},0}}{1+\delta_{\tau,0}}\right]^{1/2}|\mathbf{KR}\rangle, \tag{36}$$

with orthonormality relations

$$\langle\mathbf{K}'\boldsymbol{\tau}'|\mathbf{K}\boldsymbol{\tau}\rangle=\delta_{\mathbf{K},\mathbf{K}'}[\delta_{\tau,\tau'}+\delta_{\tau,-\tau'}][1+\delta(\boldsymbol{\tau})]^{-1}. \tag{37}$$

On inspection of Eqs. (35) and (36), we see that we can split H into a part H_0 which is diagonalizable under the transformation Eq. (36) and an interaction V in the following manner:

$$H_0|\mathbf{R}\rangle=-4S\sum_{\Delta}\cos\tfrac{1}{2}(\mathbf{K}\cdot\boldsymbol{\Delta})\left[\frac{1+\delta_{\mathbf{R},-\Delta}}{1+\delta_{\mathbf{R},0}}\right]^{1/2}|\mathbf{R}+\boldsymbol{\Delta}\rangle,$$

$$V|\mathbf{R}\rangle=-2\delta_{\mathbf{R}\Delta}|\mathbf{R}\rangle+4S\sum_{\Delta}\cos\tfrac{1}{2}(\mathbf{K}\cdot\boldsymbol{\Delta})\left[\frac{1+\delta_{R,-\Delta}}{1+\delta_{R,0}}\right]^{1/2} \times\left\{1-\left(1-\frac{\delta_{\mathbf{R},0}}{2S}\right)^{1/2}\left(1-\frac{\delta_{\mathbf{R},-\Delta}}{2S}\right)^{1/2}\right\}|\mathbf{R}+\boldsymbol{\Delta}\rangle. \tag{38}$$

When we apply the transformation Eq. (36) to H_0 we get the energy eigenvalue (energy of two free spin waves)

$$H_0|\boldsymbol{\tau}\rangle=\{-4S\textstyle\sum_{\Delta}\cos\frac{1}{2}(\mathbf{K}\cdot\boldsymbol{\Delta})\cos\boldsymbol{\tau}\cdot\boldsymbol{\Delta}\}|\boldsymbol{\tau}\rangle =E_{\tau}^{\mathbf{K}}|\boldsymbol{\tau}\rangle. \tag{39}$$

The eigenfunctions of H_0 in terms of the mixed basis are

$$u_{\tau}^{\mathbf{K}}(\mathbf{R})=[N(1+\delta_{\mathbf{R},0})(1+\delta_{\tau,0})]^{-1/2}\sqrt{2}\cos\boldsymbol{\tau}\cdot\mathbf{R}. \tag{40}$$

Remember on comparing this to Eq. (36) that $\mathbf{R}$ and $-\mathbf{R}$ specify the same state, and we must not count the same state twice.

The nonzero matrix elements of the perturbation V in terms of the mixed basis are

$$V_{\Delta\Delta}=-2,$$
$$V_{0\Delta}=V_{\Delta0}=4\sqrt{2}S\{1-(1-1/2S)^{1/2}\}\cos\tfrac{1}{2}(\mathbf{K}\cdot\boldsymbol{\Delta}). \tag{41}$$

The Green's function for our Schrödinger equation is derived in the standard fashion:

$$G=(E-H_0)^{-1}={\sum_{\lambda}}'\frac{u_{\lambda}^{\mathbf{K}}(\mathbf{R})u_{\lambda}^{\mathbf{K}*}(\mathbf{R}')}{E-E_{\lambda}^{\mathbf{K}}}, \tag{42}$$

where the prime on the summation sign indicates that we count each distinct state only once. Explicitly,

$$G_E^{\mathbf{K}}(\mathbf{R},\mathbf{R}')=[N^2(1+\delta_{R,0})(1+\delta_{R',0})]^{-1/2} \times2\sum_{\lambda}\frac{\cos\boldsymbol{\lambda}\cdot\mathbf{R}\cos\boldsymbol{\lambda}\cdot\mathbf{R}'}{E-E_{\lambda}^{\mathbf{K}}}. \tag{43}$$

The Green's function will be evaluated in an Appendix.

We now have everything necessary to solve the Lippmann-Schwinger scattering equation for the two-spin-wave problem.

CALCULATION OF EXACT EXCHANGE SCATTERING AMPLITUDE

The Lippmann-Schwinger equation is the integral equation corresponding to the Schrödinger differential equation with the boundary condition that the solutions should be scattered waves. It is conventionally written in the form

$$\Psi = u + [E - H_0 + i\epsilon]^{-1} V\Psi, \tag{44}$$

where u is an eigenfunction of $H_0 = H - V$ with energy E (usually a plane wave), and the Green's function

$$G = [E - H_0 + i\epsilon]^{-1} \tag{45}$$

is asymptotically proportional to a spherical wave for large R. A formal (and in this case practical) solution is given by

$$\Psi = u + GV(1 - GV)^{-1} u. \tag{46}$$

Since the nonvanishing part of V is only 4×4, the nonvanishing part of the matrix $V(1-GV)^{-1}$ is similarly 4×4. It is easy to perform the matrix algebra needed to calculate this matrix. The asymptotic behavior of G for large R can be found by the method of stationary phase, and is given in the appendix. Then the portion of the wave function describing the scattering is, for large R

$$\Psi_s = (1/R)[\lim_{R\to\infty}(RG)]V(1-GV)^{-1}u. \tag{47}$$

When the total wave vector $\mathbf{K}$ is on the (111) axis, the matrices G and V can be reduced to a sum of one 2×2 matrix and two 1×1 matrices. We will carry through the calculations for this special case.

Let the row and column indices 0, 1, 2, 3 stand for the values of $\mathbf{R} = \mathbf{0}$, $\hat{x}$, $\hat{y}$, $\hat{z}$, respectively. The matrices G and V are both of form

$$\Gamma = \begin{bmatrix} a & b & b & b \\ b & c & d & d \\ b & d & c & d \\ b & d & d & c \end{bmatrix}, \tag{48}$$

and can be reduced by the matrix T

$$T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 3^{-1/2} & 3^{-1/2} & 3^{-1/2} \\ 0 & 6^{-1/2} & 6^{-1/2} & -2\times 6^{1/2} \\ 0 & 2^{-1/2} & -2^{-1/2} & 0 \end{bmatrix}, \tag{49}$$

to the form

$$T\Gamma T^{-1} = \begin{bmatrix} a & \sqrt{3}b & 0 & 0 \\ \sqrt{3}b & c+2d & 0 & 0 \\ 0 & 0 & c-d & 0 \\ 0 & 0 & 0 & c-d \end{bmatrix}. \tag{50}$$

The determinant of the matrix $(1-GV)$ is

$$\mathrm{Det}(1-GV) = D_1 D_2^2, \tag{51}$$

where

$$D_1 = 1 - 6\sqrt{2}G_{01}\left(\cos\frac{K}{2\sqrt{3}} + \frac{\mathcal{E}}{3\cos(K/2\sqrt{3})}\right) \tag{52a}$$

$$D_2 = 1 - 6G_{12} - \frac{2\sqrt{2}\mathcal{E}}{\cos(K/2\sqrt{3})}G_{01}. \tag{52b}$$

In these expressions, we have defined

$$\mathcal{E} = -\cos\frac{K}{2\sqrt{3}}\sum_i \cos q_i \tag{53}$$

and $K^2 = K_x^2 + K_y^2 + K_z^2 = 3K_x^2$. We occasionally refer to the quantity $3 + \mathcal{E}/\cos(K/2\sqrt{3})$ as the relative energy. The Green's functions G_{01} and G_{12} are discussed in the Appendix. It is shown there that they can be expressed as the Fourier transform of products of three Bessel functions whose arguments depend on $\mathbf{K}$. In the case of $\mathbf{K}$ along the (111) axis, the $\mathbf{K}$ dependence may be found explicitly and removed from the integrals. The remaining objects have been tabulated elsewhere.[8] Since the determinant appears in the denominator of the inverse matrix, and hence in the denominator of the scattering amplitude, the amplitude is infinite whenever the determinant is zero. This condition determines $E(\mathbf{K})$ for bound states and scattering resonances, as will be discussed more completely in the following section.

The plane wave normalized to unit volume is

$$u = 2^{1/2}[(1+\delta_{\lambda,0})(1+\delta_{\mathbf{R},0})]^{-1/2}\cos\boldsymbol{\lambda}\cdot\mathbf{R}. \tag{54}$$

On inverting the matrix $1-GV$ and carrying out the matrix multiplication, we get the scattering amplitude

$$f = Re^{-i\mathbf{q}\cdot\mathbf{R}}\psi_S = [2^{3/2}\pi S\cos(K/2\sqrt{3})]^{-1}\left[\frac{\sum_i \sin^2 q_i}{\sum_{\mathrm{cyclic}} \sin^2 q_i \cos q_j \cos q_k}\right]^{1/2} \times\left[\frac{\mathcal{E}}{D_1}\left(1+\frac{\mathcal{E}}{3\cos^2(K/2\sqrt{3})}\right) - \frac{1}{D_2}\left(\frac{\mathcal{E}^2}{3\cos^2(K/2\sqrt{3})} - \sum_i \cos\lambda_i\cos q_i\right)\right]. \tag{55}$$

Let us look at the long-wavelength limit. There the "D-wave" contribution (which has denominator D_2) is of order λ^4 while the isotropic "S-wave" part is of order λ^2. The radical in front and D_1 are unity to lowest order. Input and output velocities will be equal in this limit, and so the total cross section will be given by

$$\sigma = 4\pi|f|^2 = \frac{[(\tfrac{1}{2}\mathbf{K}+\boldsymbol{\lambda})\cdot(\tfrac{1}{2}\mathbf{K}-\boldsymbol{\lambda})]^2}{8\pi S^2} = \frac{(\boldsymbol{\tau}\cdot\boldsymbol{\tau}')^2}{8\pi S^2}, \tag{56}$$

[8] T. Wolfram and J. Callaway, Phys. Rev. 130, 2207 (1963).

where $\boldsymbol{\tau}$ and $\boldsymbol{\tau}'$ are the wave vectors of the two spin waves. This result was obtained by Dyson[7] by a different method. It is also of interest that the scattering amplitude, Eq. (55), vanishes whenever one of the spin-wave vectors $\boldsymbol{\tau}$, $\boldsymbol{\tau}'$ goes to zero (regardless of the size of the other).

The exact scattering cross section in position is given by

$$d\sigma/d\Omega_R = V_q |f|^2/V_\lambda \tag{57}$$

since $\langle u^*u\rangle = 1$. We have

$$V_q = \cos(K/2\sqrt{3})[\sum_i \sin^2 q_i]^{1/2} \tag{58}$$

for this special case, so that

$$\frac{d\sigma}{d\Omega} = [8\pi S^2 \cos^2(K/2\sqrt{3})]^{-1} (\sum_i \sin^2 q_i)^{3/2} (\sum_i \sin^2\lambda_i)^{-1/2} (\sum_{\text{cyclic}} \sin^2 q_i \cos q_j \cos q_k)^{-1}$$
$$\times \left[\frac{\mathcal{E}}{D_1}\left(1+\frac{\mathcal{E}}{3\cos^2(K/2\sqrt{3})}\right) - \frac{1}{D_2}\left(\frac{\mathcal{E}^2}{3\cos^2(K/2\sqrt{3})} - \sum_i \cos\lambda_i \cos q_i\right)\right]^2. \tag{59}$$

BOUND STATES AND SCATTERING RESONANCES

In this section we will give a detailed discussion of the bound states and scattering resonances in one case. Although the direct observation of these spin complexes seems somewhat remote at present, the results are of some interest as an illustration of the general methods of Ref. 5. We will therefore locate the bound states and scattering resonances as a function of $\mathbf{K}$ when $\mathbf{K}$ lies along the (111) axis. The width of the resonances will also be shown. Finally, we will exhibit the cross section for energies close to the bottom of the spin wave continuum for particular values of $\mathbf{K}$. The restriction of these considerations to $\mathbf{K}$ along the (111) axis is prompted by the great simplification this produces in the equation giving the scattering amplitude.

Let us first consider the s-like states. We must evaluate D_1. From Eq. (A9) of the Appendix, we have

$$G_{01}(\mathcal{E}/a) = \frac{\sqrt{2}}{8S}\int_0^\infty \exp(i\mathcal{E}t/a) J_0^2(t) J_1(t)\,dt, \tag{60}$$

where $a=\cos K/2\sqrt{3}$. This integral may be obtained from tables given by Wolfram and Callaway.[8] Let us first note an important property. For $\mathcal{E}/a < -3$, G_{01} is real. From Eq. (53), we see that this corresponds to the bottom of the spin-wave band for the particular $\mathbf{K}$ considered. This means that the equation $D_1=0$ can be satisfied only outside of the band. Further, since the real part of G_{01} is negative near the band extrema, solutions to $D_1=0$ can occur only when $\mathcal{E}$ is negative—that is, the bound spin-wave states can only lie below, rather than above, the two-spin-wave continuum. Within this continuum, although the equation $D_1=0$ can never be satisfied, the equation $\mathrm{Re}D_1=0$ can hold for some $\mathcal{E}, K$; and in this case, there is the possibility of a scattering resonance. Similar remarks can be easily seen to apply to the d-like states for which the relevant quantity is D_2.

Although the real parts of D_1 and D_2 must be determined numerically, simple expressions can be found for the imaginary parts. It is shown in the Appendix, that if we define q_0 through

$$\tfrac{1}{2}q_0^2 = \mathcal{E}/a + 3, \tag{61}$$

that we have the following approximate expressions for the imaginary part of G_{01}:

$$\mathrm{Im}G_{01} = -(8\pi\sqrt{2}aS)^{-1}\sin q_0. \tag{62}$$

We denote the imaginary part of D_1 by $D_{1,i}$. Then

$$D_{1,i} = 6\sqrt{2}(\mathrm{Im}G_{01})[\cos(K/2\sqrt{3})-1]$$
$$\approx -\frac{3}{4\pi S}\sin q_0\left(1-\frac{1}{\cos(K/2\sqrt{3})}\right). \tag{63}$$

Hence, we see that, for fixed K, $D_{1,i}$ is proportional to q_0 for small q_0.

A similar calculation shows that $D_{2,i}$ is proportional to q_0^5 for small q_0.

The multiplicative factor under the radical in Eq. (55) can be expanded in terms of the energy for energies close to the bottom of the continuum for fixed K. We have, to first order in q_0^2, neglecting anisotropic terms

$$\left[\frac{\sum_i \sin^2 q_i}{\sum_{\text{cyclic}} \sin^2 q_i \cos q_j \cos q_k}\right]^{1/2} \approx \tfrac{1}{5}(8+\mathcal{E}/a). \tag{64}$$

We will now give numerical results fot the s-like states. The s-wave portion of the cross section, defined as $4\pi|f_s|^2$, where f_s arises from the first term of Eq. (55) is shown in Fig. 1 as a function of q_0^2 [which is defined in Eq. (61)] for several values of K. It will be observed that there are no scattering resonances in this case. Although the real part of D_1 does, under some circumstances, vanish within the continuum, the cross section does not exhibit a maximum except for $q=0$. This results from the rapid rise of the imaginary part of D_1 within the continuum. The cross section can, however, become quite large for $q=0$. This occurs for values of K such that the real part of D_1 is small at $q=0$, and therefore that a bound state is, in a certain sense, nearby. A similar phenomenon is found in nuclear physics, where

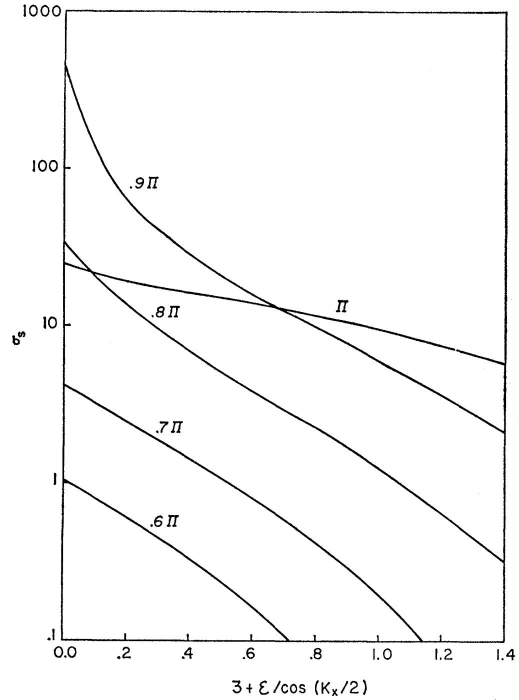

FIG. 1. The s-wave contribution to the total cross section σ_s (in units of the square of the lattice constant) is shown as a function of relative energy above the bottom of the two-body continuum. Only values of **K** along the (111) axis are considered. The curves are labeled by the value of the component of K along this axis.

the scattering amplitude for two nucleon scattering is quite large in the singlet state at zero energy as a consequence of the low-energy virtual singlet state of the deuteron.

Outside of the continuum, bound states are found for large values of K as originally predicted by Wortis[2] and Hanus.[3] A crude physical picture of such states is that of two flipped spins bound together propagating through a lattice. Computations of the energies of these bound states were based on the tabulated values of the Bessel function integrals as given by Wolfram and Callaway, and extended to large negative values of $\mathcal{E}/a$ by means of asymptotic expansions (see Appendix). The results are shown graphically in Figs. 2 and 3 for the case $S=1$.

In Fig. 2, the boundaries of the two-body continuum are shown, with the s-like and d-like bound states appearing for large values of K. At the zone boundary, the energies of these two branches coincide, and are given by $\mathcal{E}=3-1/4S$. The region containing the bound states is shown in more detail in Fig. 3. The energies of the d-like bound states depend only weakly on K. Inside the continuum, these d states become resonances whose width increases as K decreases.

A resonance has a width. General expressions for the energies and widths of resonant states are given in Ref. 5. If we consider a state of type β (belonging to the βth irreducible representation of some group; in this case, the group of the wave vector **K**), the energy of a reso-

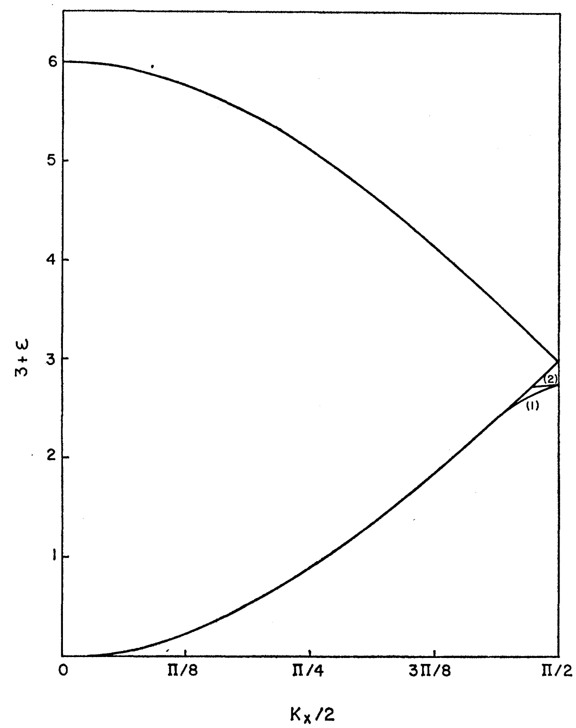

FIG. 2. The energies of the bound two-spin-wave states are shown as functions of K_x for total wave vectors lying along the (111) axis and $S=1$. The upper and lower long curves are the boundaries of the two-spin-wave continuum. The short curves (1) and (2) represent the bound states; (1) showing the s-like states and (2) showing the d-like states.

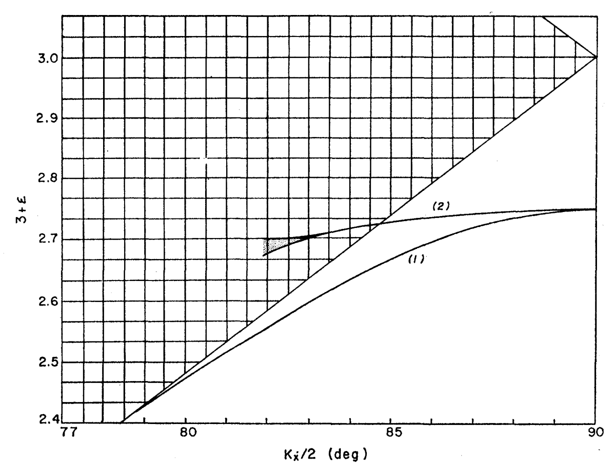

FIG. 3. The energies of the bound two-spin-wave states are shown as functions of K_x for total wave vectors along the (111) axis and $S=1$. This diagram is an enlargement of the portion of Fig. 2 containing the bound states. The cross-hatched region represents the two-body continuum. Curves (1) and (2) are the s- and d-like bound states, respectively. The d-like bound states connect with a set of resonant states in the continuum whose width is indicated schematically.

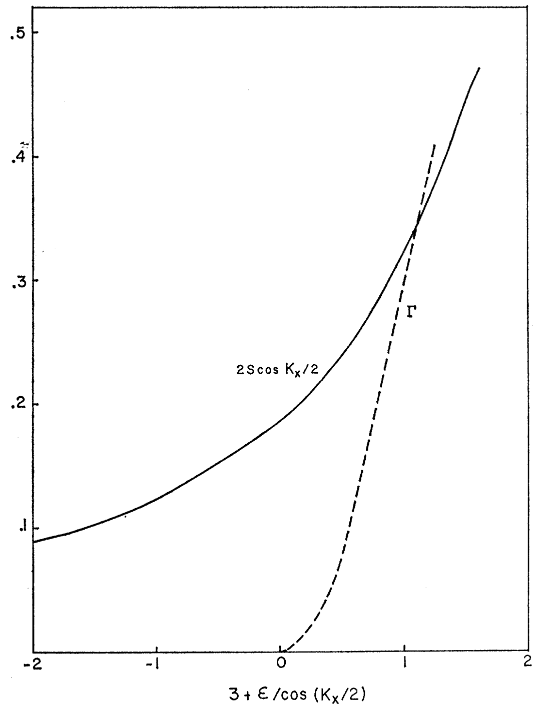

FIG. 4. The locations and widths of the d-wave bound states and resonances are shown in another representation for K along the (111) axis of the crystal. The ordinate is dimensionless. The solid curve shows values of $2S\cos K_x/2$ for which a bound state or a resonance occurs for a fixed value of the relative energy $3+\mathcal{E}/\cos(K_x/2)$ [see Eq. (53)]. The dashed curve gives values of the dimensionless width of a resonance as a function of relative energy.

nance is

$$E_{\beta,r}=E_{\beta,0}-\frac{D_{\beta,i}D_{\beta,i}'}{(D_{\beta,r}')^2+(D_{\beta,i}')^2} \tag{65}$$

and the width is

$$\Gamma_\beta=\frac{2D_{\beta,i}D_{\beta,r}'}{(D_{\beta,r}')^2+(D_{\beta,i}')^2}. \tag{66}$$

The quantities $D_{\beta,r}$ and $D_{\beta,i}$ are the real and imaginary parts of the portion of the determinant of 1-GV coming from representation β; thus, in our case, these are D_1 and D_2. The prime indicates differentation with respect to energy. The real part of the determinant D_β vanishes at an energy $E_{\beta,0}$, and it is assumed that the resonance energy is close to this; that is, the second term in Eq. (65) is small. All the D_β which appear in Eqs. (65) and (66) are evaluated at $E=E_{\beta,0}$.

The positions and widths of the d-wave resonances have been computed from these equations. As might be expected, for resonances close to the bottom of the two spin wave continuum, $D_{\beta,r}'\gg D_{\beta,i}'$. The results are shown graphically in Fig. 4. Narrow d-wave resonances are found close to the bottom of the continuum.

With respect to the question of possible experimental observation of some of the features of the two-spin-waves system, perhaps the most important of the results obtained here is the large s-wave cross section which persists to moderately large values of the relative energy. This suggests that spin-wave–spin-wave scattering may be reasonably effective in reducing the thermal conductivity of a spin-wave system below that calculated using the long-wavelength approximation. In this connection, however, it must be observed that the cross section in momentum space, rather than that in position space, is relevant for such a calculation. The two quantities are different in the case of anisotropic energy surfaces. This point is discussed in more detail in Ref. 7.

APPENDIX

Evaluation of Green's Functions

We refer to Eq. (39) for the energy eigenvalues, and to Eq. (43) for the Green's function appropriate to the two-spin-wave problem. The Green's function has also been discussed by Dyson and Wortis. The singularities of Green's functions of a similar type have been discussed elsewhere by Maradudin.[9]

The summation is replaced by an integral in the usual way. A small positive imaginary part is added to the energy in the denominator to select outgoing waves. We convert the numerator from a product of cosines to a sum of exponentials. Define some new symbols:

$$\epsilon=E/8S,\quad a_i=\cos\tfrac{1}{2}K_i. \tag{A1}$$

Then Eq. (43) for the Green's function becomes

$$G_E{}^{\mathbf{K}}(\mathbf{R},\mathbf{R}')=\frac{[(1+\delta_{\mathbf{R},0})(1+\delta_{\mathbf{R}',0})]^{-1/2}}{8S(2\pi)^3}\times\int d^3\lambda\frac{[e^{i\lambda\cdot(\mathbf{R}+\mathbf{R}')}+e^{-i\lambda\cdot(\mathbf{R}-\mathbf{R}')}]}{\mathcal{E}+\sum_i a_i\cos\lambda_i+i\epsilon}. \tag{A2}$$

The Green's function can be evaluated in terms of single integrals over triple products of Bessel functions. We make use of the identity

$$(x+i\epsilon)^{-1}=-i\int_0^\infty \exp[i(x+i\epsilon)t]dt,\quad \epsilon>0,\quad x\text{ real}, \tag{A3}$$

to move the denominator in Eq. (A2) into the exponents, permitting separation of variables in the integrand. Our Green's function can then be written in the form

$$G_E{}^{\mathbf{K}}(\mathbf{R},\mathbf{R}')=\frac{-i[(1+\delta_{R,0})(1+\delta_{R',0})]^{-1/2}}{8S(2\pi)^3}\int_0^\infty e^{i\mathcal{E}t}\times\{\prod_j I(m_j^+,a_j)+\prod_{j'} I(m_j^-,a_j)\}dt, \tag{A4}$$

[9] A. A. Maradudin, in *Phonons and Phonon Interactions*, edited by T. A. Bak (W. A. Benjamin, Inc., New York, 1964).

where

$$I(m_j,a_j)=\int_{-\pi}^{\pi}\exp[i\{m_j\lambda_j+a_jt\cos\lambda_j\}]d\lambda_j \quad \text{(A5)}$$

and we have written the integral components of the lattive vectors as

$$m_j^{\pm}=(\mathbf{R}\pm\mathbf{R}')_j. \quad \text{(A6)}$$

The integral in Eq. (A5) is proportional to a Bessel function:

$$I(m,a)=2\pi i^m J_m(at), \quad \text{(A7)}$$

and therefore

$$G_E^{\mathbf{K}}(\mathbf{R},\mathbf{R}')=(-i/8S)[(1+\delta_{\mathbf{R},0})(1+\delta_{\mathbf{R}',0})]^{-1/2}$$
$$\times\int_0^\infty \exp(i\mathcal{E}t)\{i^{\Sigma m_j^+}\prod_j J_{m_j^+}(a_j,t)$$
$$+i^{\Sigma m_j^-}\prod_j J_{m_j^-}(a_jt)\}dt. \quad \text{(A8)}$$

We now exhibit the nearest-neighbor Green's functions:

$$G_{00}=G_E^{\mathbf{K}}(0,0)=(-i/8S)\int_0^\infty \exp(i\mathcal{E}t)J_0(a_xt)\times J_0(a_yt)J_0(a_zt)dt,$$

$$G_{01}=G_E^{\mathbf{K}}(0,\mathbf{x})=(2^{1/2}/8S)\int_0^\infty \exp(i\mathcal{E}t)J_1(a_xt)\times J_0(a_yt)J_0(a_zt)dt, \quad \text{(A9)}$$

$$G_{11}=G_E^{\mathbf{K}}(\mathbf{x},\mathbf{x})=(-i/8S)\int_0^\infty \exp(i\mathcal{E}t)\times[J_0(a_x,t)-J_2(a_x,t)]J_0(a_yt)J_0(a_zt)dt,$$

$$G_{12}=G_E^{\mathbf{K}}(\mathbf{x},\mathbf{y})=(i/4S)\int_0^\infty \exp(i\mathcal{E}t)J_1(a_xt)\times J_1(a_yt)J_0(a_zt)dt,$$

and cyclic in x, y, z.

These functions are tabulated for

$$a_x=a_y=a_z=a=1. \quad \text{(A10)}$$

The identity

$$G(\mathcal{E},\mathbf{a})=(1/a)G(\mathcal{E}/a,\mathbf{1}) \quad \text{(A11)}$$

permits us to use the same tabulation to evaluate the Green's functions when the total wave vector $\mathbf{K}$ is on the (111) axis.

Asymptotic Form of the Green's Function

We shall evaluate the asymptotic form of the Green's function for large argument by the method of stationary phase, as described for instance by Callaway.[5]

The phases of the two exponentials in the integrand of Eq. (A4) are

$$\phi^{\pm}=\boldsymbol{\lambda}\cdot(\mathbf{R}\pm\mathbf{R}')+t[\mathcal{E}+\sum_j a_j\cos\lambda_j]. \quad \text{(A12)}$$

At a point of stationary phase in $\boldsymbol{\lambda}t$ space, the gradient of ϕ is zero by definition. For large R, and for $R'\ll R$, the term containing R' becomes vanishingly small relative to the others, and both phases yield the same satationary points. When we set the gradient of ϕ equal to zero in the limit of large R, we get the following equations which determine the stationary points $\mathbf{q},t_0$.

$$t_0=R(\sum_j a_j^2\sin^2 q_j)^{1/2},$$
$$\mathbf{R}/R=\hat{r}=(\sum_j a_j\sin q_j\,\hat{e}_j)(\sum_j a_j^2\sin^2 q_j)^{-1/2}, \quad \text{(A13)}$$
$$\mathcal{E}=-\sum_j a_j\cos q_j.$$

It can be shown that for a general value of the total wave vector $\mathbf{K}$, only one value of $\mathbf{q},t_0$ satisfies these equations.

We assume that the integral in Eq. (A4) for large R receives contributions only from a small neighborhood of $\mathbf{q}t_0$. We expand ϕ in this neighborhood and keep the lowest order terms. The integral is then easy to perform, yielding the asymptotic form of the Green's function:

$$G_E^{\mathbf{K}}(\mathbf{R},\mathbf{R}')=-[8\pi SR(1+\delta_{\mathbf{R}',0})^{1/2}]^{-1}e^{i\mathbf{q}\cdot\mathbf{R}}\cos\mathbf{q}\cdot\mathbf{R}'\times\left[\frac{\sum_j a_j^2\sin^2 q_j}{\sum_{\text{cyclic}} a_i^2 a_j a_k \sin^2 q_i\cos q_j\cos q_k}\right]^{1/2}, \quad \text{(A14)}$$

where $\mathbf{q}$ is the scattered relative momentum.

Imaginary Parts of the Green's Functions

It is sometimes possible to derive relatively simple expressions for the imaginary parts of the Green's functions $G_E^{\mathbf{K}}$ $(\mathbf{R},\mathbf{R}')$ for small R, R' and for energies near the bottom of the spin wave continuum for that $\mathbf{K}$. First, we observe from (A2) that, because of the inversion symmetry of the denominator with respect to $\boldsymbol{\lambda}$, the Green's function $G_E^{\mathbf{K}}$ would be real were it not for the presence of the $i\epsilon$. This indicates that we can obtain the imaginary part of $G_E^{\mathbf{K}}$ from the imaginary part of the expression

$$\lim_{\epsilon\to 0}(x+i\epsilon)^{-1}=P(1/x)-i\pi\delta(x).$$

Hence

$$\mathrm{Im}G_E^{\mathbf{K}}(\mathbf{R},\mathbf{R}')=-[64S\pi^2(1+\delta_{\mathbf{R},0})^{1/2}(1+\delta_{\mathbf{R}',0})^{1/2}]^{-1}\times\int d^3\lambda[e^{i\boldsymbol{\lambda}\cdot(\mathbf{R}+\mathbf{R}')}+e^{i\boldsymbol{\lambda}\cdot(\mathbf{R}-\mathbf{R}')}]\times\delta[\mathcal{E}+\sum a_i\cos\lambda_i]. \quad \text{(A15)}$$

We see from (A15) that the Green's function can have an imaginary part only when $\mathcal{E}$ is the spin-wave continuum. We will proceed further only for K along the (111) axis. Then put $a_1=a_2=a_3=a$; and define a parameter q_0 through

$$\tfrac{1}{2}q_0^2=(\mathcal{E}/a)+3. \tag{A16}$$

Then we have

$$\mathrm{Im}G_E^{\mathbf{K}}(\mathbf{R},\mathbf{R}')=-[64S\pi^2a(1+\delta_{\mathbf{R},0})^{1/2}(1+\delta_{\mathbf{R}',0})^{1/2}]^{-1}\times\int d^3\lambda[e^{i\lambda\cdot(\mathbf{R}+\mathbf{R}')}+e^{i\lambda\cdot(\mathbf{R}-\mathbf{R}')}]\times\delta[(\tfrac{1}{2}q_0^2)-3+\sum_i\cos\lambda_i]. \tag{A17}$$

We obtain the desired approximation by expanding the cosines in powers of λ. We have, to fourth order

$$3-\sum_i\cos\lambda_i=\tfrac{1}{2}\lambda^2-(1/40)\lambda^4-(1/24)\times(\lambda_x^4+\lambda_y^4+\lambda_z^4-\tfrac{3}{5}\lambda^4). \tag{A18}$$

The third term in (A18) is the leading term of cubic rather than spherical symmetry. We neglect this term, together with all contributions of order λ^6 and higher. We may then integrate over angles, obtaining

$$\mathrm{Im}G_E^{\mathbf{K}}(\mathbf{R},\mathbf{R}')=-[8\pi Sa(1+\delta_{\mathbf{R},0})^{1/2}(1+\delta_{\mathbf{R}',0})^{1/2}]^{-1}\times\int d\lambda\cdot\lambda\left[\frac{\sin\lambda|\mathbf{R}+\mathbf{R}'|}{|\mathbf{R}+\mathbf{R}'|}+\frac{\sin\lambda|\mathbf{R}-\mathbf{R}'|}{|R-R'|}\right]\times\delta(q_0^2-\lambda^2+\lambda^4/20). \tag{A19}$$

The integration over λ may now be performed, yielding to order q^4.

$$\mathrm{Im}G_E^{\mathbf{K}}(\mathbf{R},\mathbf{R}')=-[16\pi Sa(1+\delta_{\mathbf{R},0})^{1/2}(1+\delta_{\mathbf{R}',0})^{1/2}]^{-1}\times(1+q_0^2/10)\left\{\frac{\sin[q_0(1+q_0^2/40)|\mathbf{R}+\mathbf{R}'|]}{|\mathbf{R}+\mathbf{R}'|}+\frac{\sin[q_0(1+q_0^2/40)|\mathbf{R}-\mathbf{R}'|]}{|\mathbf{R}-\mathbf{R}'|}\right\}. \tag{A20a}$$

If the terms in q_0^2 are neglected, we have the first approximation

$$\mathrm{Im}G_E^{\mathbf{K}}(\mathbf{R},\mathbf{R}')=-[16\pi Sa(1+\delta_{\mathbf{R},0})^{1/2}(1+\delta_{\mathbf{R}',0})^{1/2}]^{-1}\times\left[\frac{\sin q_0|\mathbf{R}+\mathbf{R}'|}{|\mathbf{R}+\mathbf{R}'|}+\frac{\sin q_0|\mathbf{R}-\mathbf{R}'|}{|\mathbf{R}-\mathbf{R}'|}\right]. \tag{A20b}$$

It should be noted that the approximations here involve the size of q_0 rather than the size of q_0R.

Green's Functions for Energies Below the Continuum

Expressions for the Green's functions for energies below the two-spin-wave continuum and a small can be obtained by the following device. We illustrate for the case of G_{01}, and it is readily apparent how the procedure may be applied to the other functions. We consider only the case in which $\mathbf{K}$ is parallel to the (111) axis.

With the use of (A11), we have

$$G_{01}=\frac{2^{1/2}}{8Sa}\int_0^\infty e^{i\mathcal{E}t/a}J_1(t)J_0^2(t)dt. \tag{A21}$$

Put $\mathcal{E}/a=-w$, $it=z$. Then for $w>3$, we can write

$$G_{01}=-\frac{2^{1/2}}{8Sa}\int_0^\infty e^{-wz}I_1(z)I_0^2(z)dz, \tag{A22}$$

in which I_0, I_1 are Bessel functions of imaginary argument. An asymptotic expansion of G_{01} in decreasing powers of W is generated by expanding the Bessel functions in increasing powers of z:

$$I_n(z)=\sum_{r=0}^\infty\frac{(z/2)^{n+2r}}{r!(n+r)!}.$$

A straightforward calculation shows that

$$G_{01}=\frac{1}{8\sqrt{2}aw^2}\left[1+\frac{15}{4w^2}+\frac{155}{8w^4}+\cdots\right]. \tag{A23}$$

Knowledge of G_{01} suffices for the evaluation of D_1. To evaluate D_2 in this limit requires an expansion for G_{12}. By the same method, we have

$$G_{12}=-\frac{1}{4Sa}\int_0^\infty e^{-wz}I_1^2(z)I_0(z)dz,$$

$$=-\frac{1}{8Saw^3}\left[1+\frac{6}{w^2}+\frac{75}{2w^4}+\cdots\right]. \tag{A24}$$