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Two-Spin-Wave Resonances and the Analyticity of the t Matrix in the Heisenberg Ferromagnet*

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We consider the scattering of two spin waves in a simple cubic Heisenberg ferromagnet with nearest-neighbor interaction at zero temperature. The analytic properties of the integrals relevant to the bound-state problem are examined and the solutions to the bound-state conditions are located in the complex energy (ω) plane for the first time. It is found that, as a function of ω, there are two Riemann sheets near the bottom of the two-spin-wave band. For total wave vector $\vec{q}$ less than the threshold value for bound states, the existence of the d-wave resonant states discovered by Boyd and Callaway is reaffirmed. Furthermore, we confirm the observation of Boyd and Callaway that no s-wave scattering resonance exists.

I. INTRODUCTION

It has been shown by Dyson[1] that two spin waves in a Heisenberg ferromagnet interact via an attractive potential which increases with the total wave vector $\vec{q}$ of the pair. Bound or resonant states of two spin waves may exist for large $\vec{q}$. The two-spin-wave bound-state conditions have been obtained by Hanus[2] and by Wortis.[3] Later, Boyd and Callaway[4] and Silberglitt and Harris[5] obtained the same conditions by different methods. Wortis[3] has discussed the bound states in great detail. He found that, for total wave vector $\vec{q}$ larger than a threshold, there are three bound states below the two-spin-wave band, among which two states are degenerate if $\vec{q}$ is in the [111] direction. Boyd and Callaway[4] derived an expression for the two-spin-wave scattering cross section for $\vec{q}$ along the [111] direction, which they resolved into two partial-wave components, s and d waves. They showed that both s- and d-wave bound states exist, and that the d-wave state is doubly degenerate, while the s-wave state is nondegenerate. Furthermore, they pointed out that the d-wave bound states connect to resonant scattering states in the band as q passes the threshold, while the s-wave states do not show resonant behavior.[6] Looking into the singularities of the two-spin-wave t matrix, Silberglitt and Harris[5] obtained a two-spin-wave spectrum which agrees with the results of Hanus,[2] Wortis,[3] and Boyd and Callaway.[4] They also gave a physical reason why there is a d-wave resonance but no resonant s state, and investigated the effect of the d-wave resonance on the single-spin-wave spectrum.

The purpose of this paper is to reaffirm the existence of the d-wave resonance and to confirm the nonexistence of the s-wave resonance by examining the analytic properties of the integrals relevant to the bound-state problem and locating the solutions to the s- and d-wave bound-state conditions in the complex energy plane. We find that there are two Riemann sheets near the bottom of the continuum. On the physical sheet the d-wave bound-state condition is satisfied by the real energies corresponding to bound states below the band for total wave vector q larger than a threshold value q_c. For $q = q_c$ these bound-state energies connect to the complex solutions within the continuum on the unphysical sheet. These solutions are associated with resonances. The real parts of the complex solutions are the resonant state energies and the imaginary parts the widths of the resonances. Both increase as q decreases from q_c; the ratio of their increments is proportional to $(\cos\frac{1}{2}q - \cos\frac{1}{2}q_c)^{3/2}$ for $q \lesssim q_c$. So, narrow d-wave resonances are found near the bottom of the band in agreement with the results of Boyd and Callaway.[4] For q larger than a threshold value q_c', the s-wave bound-state condition has real energy solutions corresponding to bound states below the continuum on the physical sheet. When $q < q_c'$, however, *there exist only real solutions which are below the continuum on the unphysical sheet;* they move toward the band bottom as q increases, and connect to the bound-state energies for $q = q_c'$. Therefore, there is no s-wave resonance.

In this paper, we study the analytic properties of the two-spin-wave t matrix by use of an approximation scheme which (a) simplifies numerical calculations but leaves the order of magnitude of the quantitative results unchanged, (b) preserves the analytic properties near the bottom of band, and (c) maintains the qualitative features of the q dependence of the solutions to the bound-state conditions.

II. BOUND-STATE CONDITIONS

An isotropic Heisenberg ferromagnet with nearest-neighbor interaction is described by the Hamiltonian

$$H = -\frac{J}{2} \sum_{\vec{i},\vec{\delta}} \vec{S}_{\vec{i}} \cdot \vec{S}_{\vec{i}+\vec{\delta}} \quad , \tag{1}$$

where the exchange coupling constant J is positive and the sum extends over all lattice vectors $\vec{i}$ and over the vectors $\vec{\delta}$ joining an atom to its z nearest neighbors. For the simple cubic lattice, $z = 6$. In this system, a simple spin wave[7] with wave vector $\vec{k}$ possesses the energy $\epsilon_K = 2JS\sum_{i=x,y,z} \times(1-\cos k_i)$ at zero temperature, with S being the lattice spin. Two spin waves, however, interact[1] via an attractive and wave-vector-dependent potential

$$V(\vec{k}_1, \vec{k}_2, \vec{q}) = -2J \sum_{i=x,y,z} \cos k_{1i}(\cos k_{2i} - \cos\tfrac{1}{2}q_i) \quad , \tag{2}$$

where $\vec{k}_1$ and $\vec{k}_2$ are, respectively, the incident and outgoing relative wave vectors, and $\vec{q}$ is the total wave vector of the pair. Following Silberglitt and Harris,[5] the two-spin-wave t matrix is

$$t(\vec{k}_1, \vec{k}_2, \vec{q}, \omega) = -2J \sum_{i,j=x,y,z} \{\cos k_{1i}(\cos k_{2j} - \cos\tfrac{1}{2}q_j) \times[1 - 2A(\vec{q}, \omega)]^{-1}_{ij}\} \ . \tag{3}$$

Here the matrix A is defined by

$$A_{ij}(\vec{q}, \omega) = -\frac{J}{8\pi^3} \iiint_{-\pi}^{\pi} \frac{\cos k_i(\cos k_j - \cos\frac{1}{2}q_j)}{\omega - \epsilon_{q/2+k} - \epsilon_{q/2-k}} \times dk_x dk_y dk_z \ , \tag{4}$$

where ω is the total energy of the interacting pair of spin waves. For $\vec{q}$ in the [111] direction,

$$(1-2A)^{-1} = \frac{1}{3(1-2A_0-4A_0')} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} + \frac{1}{3(1-2A_0+2A_0')} \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} . \tag{5}$$

The bound-state conditions[2-5] are

$$d \text{ wave:} \quad 1 - 2A_0 + 2A_0' = 0 \ , \tag{6a}$$

$$s \text{ wave:} \quad 1 - 2A_0 - 4A_0' = 0 \ . \tag{6b}$$

In the above,

$$A_0 \equiv A_{ii} = -\frac{1}{32\pi^3 S} \iiint_{-\pi}^{\pi} \frac{\cos^2 k_x - \alpha\cos k_x}{\nu + \alpha(\cos k_x + \cos k_y + \cos k_z)} \times dk_x dk_y dk_z \tag{7a}$$

and

$$A_0' \equiv A_{ij} = -\frac{1}{32\pi^3 S} \iiint_{-\pi}^{\pi} \frac{\cos k_x \cos k_y - \alpha\cos k_x}{\nu + \alpha(\cos k_x + \cos k_y + \cos k_z)} \times dk_x dk_y dk_z \ , \tag{7b}$$

with $\nu = 3(\omega/2JzS - 1)$ and $\alpha = \cos\frac{1}{2}q$. Here q is the magnitude of each component of $\vec{q}$. In order to avoid extensive numerical calculations, we approximate A_0 and A_0' by the expressions B_0 and B_0', respectively, defined by

$$B_0 = -\frac{1}{8\pi^2 S} \int_0^\pi k^2 dk \frac{R(k) - T(k)}{\nu + \alpha F(k)} \tag{8a}$$

and

$$B_0' = -\frac{1}{8\pi^2 S} \int_0^\pi k^2 dk \frac{M(k) - \alpha T(k)}{\nu + \alpha F(k)} \ , \tag{8b}$$

where

$$F(k)=3-4k^2/\pi^2 \qquad \text{for } k\le \tfrac{1}{2}\pi \tag{9a}$$

$$=1+4(\pi-k)^2/\pi^2 \quad \text{for } \tfrac{1}{2}\pi\le k\le\pi \tag{9b}$$

and

$$R(k)=\langle\cos^2(k\cos\theta)\rangle=\tfrac{1}{2}+(\sin 2k)/4k\ , \tag{10}$$

$$M(k)=\langle\cos(k\sin\theta\cos\phi)\cos(k\cos\theta)\rangle$$

$$=(\sin\sqrt{2}k)/\sqrt{2}k\ , \tag{11}$$

$$T(k)=\langle\cos(k\cos\theta)\rangle=(\sin k)/k\ . \tag{12}$$

In Eqs. (10)–(12), $\langle\rangle$ denotes the average over the solid angle Ω.[8] In Appendix A, we discuss this approximation in detail. With Eqs. (9)–(12), direct integration yields the following results:

$$\frac{1}{2\pi^2}\int_0^\pi k^2dk\,\frac{R(k)}{\nu+\alpha F(k)}=\frac{1}{64\alpha}\left[\pi z^{1/2}\ln\left(\frac{z^{1/2}+1}{z^{1/2}-1}\right)-4\pi\ln\left(\frac{a-1}{a}\right)-\frac{\pi(a+4)}{a^{1/2}}\ln\left(\frac{a^{1/2}+1}{a^{1/2}-1}\right)+H(z;2)-H(a;2)+\frac{2}{a^{1/2}}L(a;2)\right]\ , \tag{13a}$$

$$\frac{1}{2\pi^2}\int_0^\pi k^2dk\,\frac{T(k)}{\nu+\alpha F(k)}=\frac{1}{16\alpha}\left[H(z;1)+H(a;1)-\frac{2}{a^{1/2}}L(a;1)\right]\ , \tag{13b}$$

$$\frac{1}{2\pi^2}\int_0^\pi k^2dk\,\frac{M(k)}{\nu+\alpha F(k)}=\frac{1}{16\sqrt{2}\alpha}\left\{H(z;\sqrt{2})+\cos(\sqrt{2}\pi)\left[-H(a;\sqrt{2})+\frac{2}{a^{1/2}}L(a;\sqrt{2})\right]+\sin(\sqrt{2}\pi)\left[N(a;\sqrt{2})+\frac{2}{a^{1/2}}G(a;\sqrt{2})\right]\right\}\ . \tag{13c}$$

In Eq. (13),

$$\begin{aligned}H(a;c)&=\cos(\tfrac{1}{2}\pi c\,a^{1/2})\,T(a;c)-\sin(\tfrac{1}{2}\pi c\,a^{1/2})\,W(a;c)\ ,\\ G(a;c)&=\sin(\tfrac{1}{2}\pi c\,a^{1/2})\,T(a;c)+\cos(\tfrac{1}{2}\pi c\,a^{1/2})\,W(a;c)\ ,\\ N(a;c)&=-\sin(\tfrac{1}{2}\pi c\,a^{1/2})\,U(a;c)-\cos(\tfrac{1}{2}\pi c\,a^{1/2})\,V(a;c)\ ,\\ L(a;c)&=\cos(\tfrac{1}{2}\pi c\,a^{1/2})\,U(a;c)-\sin(\tfrac{1}{2}\pi c\,a^{1/2})\,V(a,c)\ ,\end{aligned} \tag{14}$$

where[9]

$$\begin{aligned}T(a;c)&=\mathrm{Si}[\tfrac{1}{2}\pi c(a^{1/2}-1)]-\mathrm{Si}[\tfrac{1}{2}\pi c(a^{1/2}+1)]\ ,\\ W(a;c)&=\mathrm{Ci}[\tfrac{1}{2}\pi c(a^{1/2}-1)]-\mathrm{Ci}[\tfrac{1}{2}\pi c(a^{1/2}+1)]\ ,\\ U(a;c)&=\mathrm{Si}[\tfrac{1}{2}\pi c(a^{1/2}-1)]+\mathrm{Si}[\tfrac{1}{2}\pi c(a^{1/2}+1)]-2\,\mathrm{Si}(\tfrac{1}{2}\pi c\,a^{1/2})\ ,\\ V(a;c)&=\mathrm{Ci}[\tfrac{1}{2}\pi c(a^{1/2}-1)]+\mathrm{Ci}[\tfrac{1}{2}\pi c(a^{1/2}+1)]-2\,\mathrm{Ci}(\tfrac{1}{2}\pi c\,a^{1/2})\ ,\end{aligned} \tag{15}$$

with

$$z=\nu/\alpha+3,\quad a=-(\nu/\alpha+1)\ . \tag{16}$$

III. SOLUTIONS AND PROPERTIES OF BOUND-STATE EQUATIONS

In Appendix B we show that for the true integrals A_0 and A_0' in the ν/α plane, there are four square-root branch points $\nu/\alpha=-3,-1,1,3$, and furthermore, for $\mathrm{Re}(\nu/\alpha)<-1$, there are two Riemann sheets cut by the real axis between -3 and -1. From (13), we see that the nonanalytic contributions in B_0 and B_0' are of the forms

$$z^{1/2}\ln\frac{z^{1/2}+1}{z^{1/2}-1}\ ,\quad (2-z)^{1/2}\ln\frac{(2-z)^{1/2}+1}{(2-z)^{1/2}-1}\ ,$$

$$\ln\frac{1-z}{2-z}\ .$$

Thus there are three branch points $z=0,1,2$ in the z plane. The cut between $z=0$ and 1 is of second order, and the cut between $z=1$ and 2 is of infinite order. Therefore, for both B_0 and B_0' in the ν/α plane with $\mathrm{Re}(\nu/\alpha)<-2$ there are two

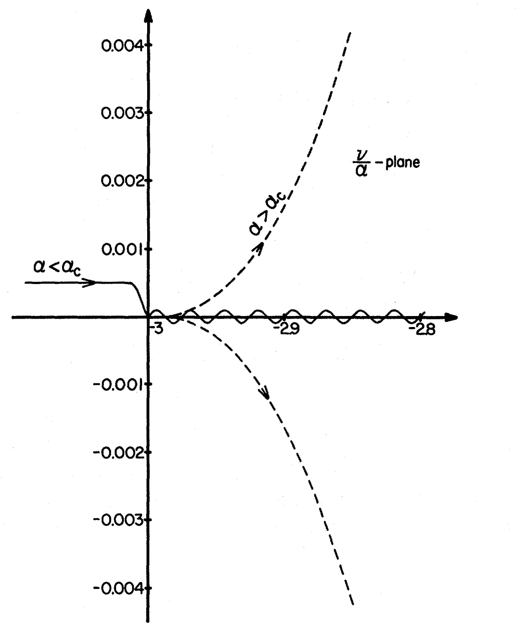

FIG. 1. Location of solutions to the d-wave bound-state condition in the ν/α plane. The solid line with arrow represents the real solutions on the first sheet. The broken lines represent the complex-conjugate solutions on the second sheet. The arrows indicate the direction of increasing α. The branch cut is represented by the wavy line.

Riemann sheets. Since $\mathrm{Re}(\nu/\alpha) = -3$ corresponds to the bottom of the two-spin-wave band, it is confirmed that near the bottom of the continuum the analytic properties of the true integrals are represented correctly in the approximated integrals.

The approximated bound-state condition for the d-wave case is

$$1 - 2B_0 + 2B_0' = 0. \tag{17}$$

Using Eqs. (7) and (8), Eq. (17) can be written in the form

$$\alpha = -\frac{1}{4\pi^2 S}\int_0^\pi k^2 dk\, \frac{R(k) - M(k)}{\nu/\alpha + F(k)} \quad . \tag{18}$$

When $\nu/\alpha \sim -3$, using (13a) and (13c), we expand the right-hand side of Eq. (18) in a power series in $z = \nu/\alpha + 3$ and write (18) as

$$S\alpha = 0.07 + 0.05z + 0.04z^2 + 0.03iz^{5/2} \quad \text{for } z \sim 0. \tag{19}$$

Letting $z = re^{i\theta}$, Eq. (19) becomes

$$S\alpha = 0.07 + 0.05r\cos\theta + 0.04r^2\cos 2\theta - 0.03r^{5/2}\sin\tfrac{5}{2}\theta\ , \tag{20a}$$

$$0 = 0.05r\sin\theta + 0.04r^2\sin 2\theta + 0.03r^{5/2}\cos\tfrac{5}{2}\theta \tag{20b}$$

for $r \sim 0$ and $4\pi \geq \theta \geq 0$. Here $2\pi \geq \theta \geq 0$ corresponds to the first sheet and $4\pi \geq \theta \geq 2\pi$ to the second sheet. We shall solve for ν/α in terms of α where $1 > \alpha \geq 0$. Solving Eq. (20), we find the following.

(i) $\nu/\alpha = -3$ when $\alpha = \alpha_c = 0.14$ for $S = \frac{1}{2}$, 0.07 for $S = 1$. Then the threshold wave vector is $q_c = 164°$ for $S = \frac{1}{2}$, $172°$ for $S = 1$.

(ii) There does not exist any solution to (20) for $\frac{1}{2}\pi \geq \theta \geq 0$, $2\pi \geq \theta \geq \frac{3}{2}\pi$, and $\frac{7}{2}\pi \geq \theta \geq \frac{5}{2}\pi$. That is, within the continuum on the first sheet and below the band on the second sheet, solutions for ν/α do not exist.

(iii) For $\frac{3}{2}\pi \geq \theta \geq \frac{1}{2}\pi$, the solutions to (20) lie on the real axis, i.e., $\theta = \pi$ and $r \propto \alpha_c - \alpha$ for $\alpha \lesssim \alpha_c$. Hence below the continuum on the first sheet there exist real solutions for ν/α for $\alpha < \alpha_c$ which move toward the band bottom as α increases.

(iv) For $\frac{5}{2}\pi \geq \theta > 2\pi$ and $4\pi > \theta \geq \frac{7}{2}\pi$, $r \propto \alpha - \alpha_c$, $\theta = 2\pi^+$ and $4\pi^-$, and

$$|r\sin\theta| \propto (\alpha - \alpha_c)^{5/2}, \quad \frac{\partial(r\sin\theta)}{\partial(r\cos\theta)} \propto (\alpha - \alpha_c)^{3/2} \quad \text{for } \alpha \gtrsim \alpha_c\ .$$

Therefore, on the second sheet within the band there are pairs of complex-conjugate solutions for ν/α for $\alpha > \alpha_c$ which move deeper into the band and farther away from the cut as α increases, and the slope of their locus is proportional to $(\alpha - \alpha_c)^{3/2}$ for $\alpha \gtrsim \alpha_c$.

From (18), we note the nonexistence of the solution for ν/α on the right half of the ν/α plane. Furthermore, only real solutions for ν/α exist below the continuum. They approach -3 from minus infinity as α increases from zero up to α_c, since

$$\frac{\partial\alpha}{\partial(\nu/\alpha)} = \frac{1}{4\pi^2 S}\int_0^\pi k^2 dk\, \frac{R(k) - M(k)}{[\nu/\alpha + F(k)]^2} > 0\ .$$

These real solutions must lie on the first sheet, which is usually called the physical sheet. The second sheet is often called the unphysical sheet. Figure 1 shows the above results.

The s-wave bound-state condition is

$$1 - 2B_0 - 4B_0' = 0\ . \tag{21}$$

By (7) and (8), Eq. (21) is written as

$$\alpha = \frac{1}{2\pi^2}\int_0^\pi k^2 dk\, \frac{R(k) + 2M(k)}{\nu/\alpha + F(k)} \Bigg/ \left(-2S + \frac{3}{2\pi^2}\int_0^\pi k^2 dk\, \frac{T(k)}{\nu/\alpha + F(k)}\right) \quad . \tag{22}$$

When $\mathrm{Re}(\nu) \geq 0$, there is no solution for ν/α to (22) for $\alpha \geq 0$, since the right-hand side of (22) is negative for $S \geq \frac{1}{2}$. Now we expand both the numerator and demominator of the right-hand side of (22) in a power series in $z=\nu/\alpha+3$, and write (22) in the following form:

$$0.3-(S+0.4)\alpha-(0.5-0.35\alpha)z+0.46(1-\alpha)iz^{1/2}=0 \quad \text{for } z\sim 0. \qquad (23)$$

With $z=re^{i\theta}$, (23) becomes, for $r\sim 0$ and $4\pi\geq\theta\geq 0$,

$$0.3-(S+0.4)\alpha-(0.5-0.35\alpha)r\cos\theta-0.46(1-\alpha)r^{1/2}\sin\tfrac{1}{2}\theta=0 \qquad (24a)$$

and

$$(0.5-0.35\alpha)r\sin\theta-0.46(1-\alpha)r^{1/2}\cos\tfrac{1}{2}\theta=0. \qquad (24b)$$

Solving (24), we find that (1) $\nu/\alpha=-3$ when $\alpha=\alpha_c'=0.32$ for $S=\frac{1}{2}$, 0.2 for $S=1$. So, the threshold wave vector is $q_c'=142°$ for $S=\frac{1}{2}$, 157° for $S=1$. (2) There is no solution on both sheets within the band for $\alpha>\alpha_c'$. (For $\frac{1}{2}\pi\geq\theta\geq 0$, $\frac{5}{2}\pi\geq\theta\geq\frac{3}{2}\pi$, $4\pi\geq\theta\geq\frac{7}{2}\pi$, no solution for r, θ exists.) (3) When $\alpha\lesssim\alpha_c'$, $\theta=\pi$ and $r\propto[(\alpha-\alpha_c')/(1-\alpha)]^2$. That is, below the band on the first sheet there exist real solutions which approach the band edge as α is raised up to α_c'. (4) When $\alpha\gtrsim\alpha_c'$, $\theta=3\pi$ and $r\propto[(\alpha-\alpha_c')/(1-\alpha)]^2$. Thus, real solutions on the second sheet below the continuum exist, and move away from band edge as α increases. The above features are shown in Fig. 2.

IV. DISCUSSION

We have explicitly shown that as q exceeds the threshold value q_c the real energy solutions to the d-wave bound-state condition (17) below the band on the physical sheet move into the band on the unphysical sheet and become complex with real and imaginary parts increasing by amounts proportional to $(\cos\frac{1}{2}q-\cos\frac{1}{2}q_c)$ and $(\cos\frac{1}{2}q-\cos\frac{1}{2}q_c)^{5/2}$, respectively. The real energies correspond to bound states of two spin waves and the complex ones are associated with the resonant scattering states. So, we have found sharp d-wave resonances close to the bottom of the continuum. For the s-wave case the bound-state solutions to Eq. (21) on the physical sheet, however, move onto the unphysical sheet, but turn back along the real axis away from the band bottom as q passes q_c'. Thus we conclude that there is no s-wave resonance. Figure 3 shows, as a comparison, the two-spin-wave spectrum by our approximation method and the results by the previous authors.[2–5] Note that the qualitive features of q or α dependence of the s- and d-wave bound-state spectra are not affected by the approximation scheme we used. The quantitative results, however, are changed by a factor of 2; the order of magnitude of the bound-state and resonant-state energies are preserved. We have avoided using computer calculation to get the exact spectrum and believe that the approximation used leads to a good understanding of the d- and s-wave properties.

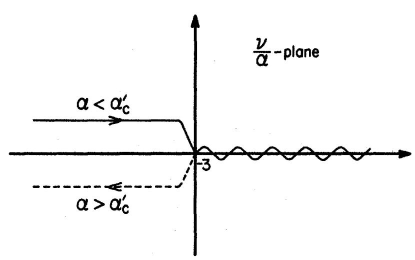

FIG. 2. s-wave case. The solid line with arrow represents the real energy solutions on the first sheet corresponding to bound states. The broken line shows the real solutions on the second sheet which do not have any physical meaning. The arrows indicate the direction of increasing α (decreasing q). The wavy line represents the branch cut.

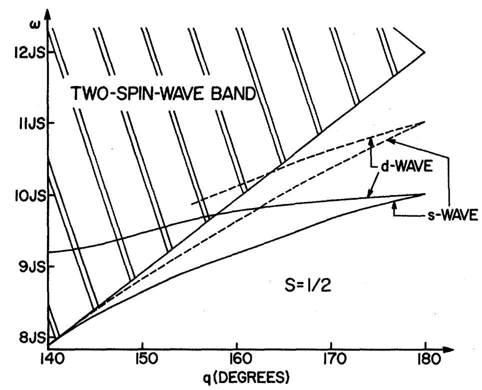

FIG. 3. The dotted lines represent the results we obtain by using the approximation method described in the text. The solid lines represent the results of previous authors. The d-wave states move into the band and show resonance. The s-wave states do not go into the band at all.

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APPENDIX A: APPROXIMATION SCHEME

In this appendix, we discuss the approximation scheme in detail. Firstly, leaving the integrand numerators of the true integrals A_0 and A_0' untouched, we approximate the cosine functions in the integrand denominators by quadratic functions f given by

$$f(y)=1-4y^2/\pi^2 \qquad \text{for } |y|\le\tfrac{1}{2}\pi$$
$$=-1+4(\pi-|y|)^2/\pi^2 \quad \text{for } \tfrac{1}{2}\pi\le|y|\le\pi\,. \qquad \text{(A1)}$$

$f(y)\simeq\cos y$ as shown in Fig. 4. Secondly, with the coordinate transformation

$$k_x=k\cos\theta\,,$$
$$k_y=k\sin\theta\cos\phi\,,$$
$$k_z=k\sin\theta\sin\phi\,, \qquad \text{(A2)}$$

we replace the cubic integration domain in the A's by a sphere of radius π centered at the origin of $\vec{k}$ space (see Fig. 5.). That is, we take the following expressions:

$$-\frac{1}{32\pi^3 S}\int_0^\pi k^2dk\int_0^{2\pi}d\phi\int_0^\pi\sin\theta\,d\theta\,\frac{\cos^2(k\cos\theta)-\alpha\cos(k\cos\theta)}{\nu+\alpha h(k,\theta,\phi)} \qquad \text{for } A_0 \qquad \text{(A3)}$$

and

$$-\frac{1}{32\pi^3 S}\int_0^\pi k^2dk\int_0^{2\pi}d\phi\int_0^\pi\sin\theta\,d\theta\,\frac{\cos(k\cos\theta)\cos(k\sin\theta\cos\phi)-\alpha\cos(k\cos\theta)}{\nu+\alpha h(k,\theta,\phi)} \qquad \text{for } A_0'\,, \qquad \text{(A4)}$$

where

$$h(k,\theta,\phi)=f(k\cos\theta)+f(k\sin\theta\cos\phi)+f(k\sin\theta\sin\phi)\,. \qquad \text{(A5)}$$

We note that (i) when $k\le\frac{1}{2}\pi$,

$$h(k,\theta,\phi)=3-4k^2/\pi^2\equiv F(k)\,, \qquad \text{(A6)}$$

and (ii) when $\frac{1}{2}\pi\le k\le\pi$, $h(k,\theta,\phi)$ is equal to or of the order of

$$1+4[(\pi-k|\cos\theta|)^2-k^2\sin^2\theta]/\pi^2$$
$$\text{for } 0\le\theta\le\tfrac{1}{4}\pi,\ \tfrac{3}{4}\pi\le\theta\le\pi,\ \text{and } 0\le\phi\le2\pi\,, \qquad \text{(A7)}$$

$$1+4[-k^2\cos^2\theta+(\pi-k|\sin\theta\cos\phi|)^2-k^2\sin^2\theta\sin^2\phi]/\pi^2$$
$$\text{for } \tfrac{1}{4}\pi\le\theta\le\tfrac{3}{4}\pi,\ 0\le\phi\le\tfrac{1}{4}\pi,\ \tfrac{3}{4}\pi\le\phi\le\tfrac{5}{4}\pi,\ \text{and } \tfrac{7}{4}\pi\le\phi\le2\pi\,, \qquad \text{(A8)}$$

$$1+4[-k^2\cos^2\theta-k^2\sin^2\theta\cos^2\phi+(\pi-k|\sin\theta\sin\phi|)^2]/\pi^2$$
$$\text{for } \tfrac{1}{4}\pi\le\theta\le\tfrac{3}{4}\pi,\ \tfrac{1}{4}\pi\le\phi\le\tfrac{3}{4}\pi,\ \text{and } \tfrac{5}{4}\pi\le\phi\le\tfrac{7}{4}\pi\,. \qquad \text{(A9)}$$

Thirdly, in order to approximate $h(k,\theta,\phi)$ by an angular-independent expression over the entire shell region, we choose the value at $\theta=\phi=0$ for (A7), at $\theta=\frac{1}{2}\pi$, $\phi=0$ for (A8), and at $\theta=\phi=\frac{1}{2}\pi$ for (A9), and obtain the final approximate form $F(k)=1+4(\pi-k)^2/\pi^2$ for $h(k,\theta,\phi)$ for $\frac{1}{2}\pi\le k\le\pi$. Thus we find expressions B_0 and B_0' defined in (7) and (8) as the approximations to A_0 and A_0', respectively.

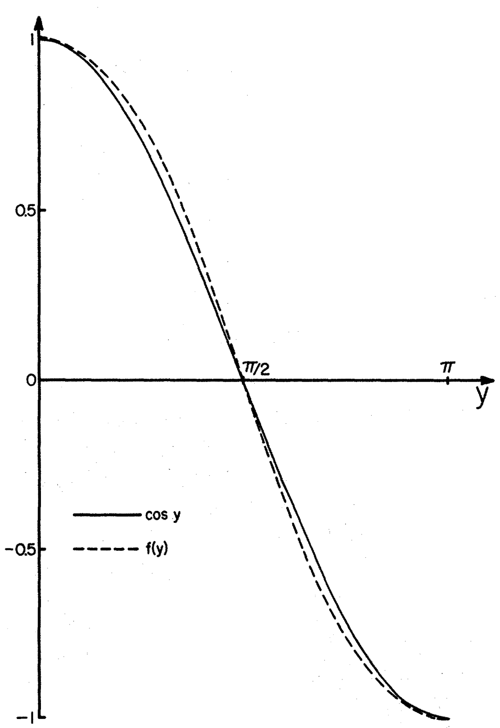

FIG. 4. cos$y$ and $f(y)$ defined in Appendix A.

APPENDIX B: ANALYTIC PROPERTIES OF TRUE INTEGRALS

We note that the singularities of the integrands of the true integrals A_0 and A_0' are given by the equation

$$\nu/\alpha+\cos k_x+\cos k_y+\cos k_z=0\,, \qquad \text{(B1)}$$

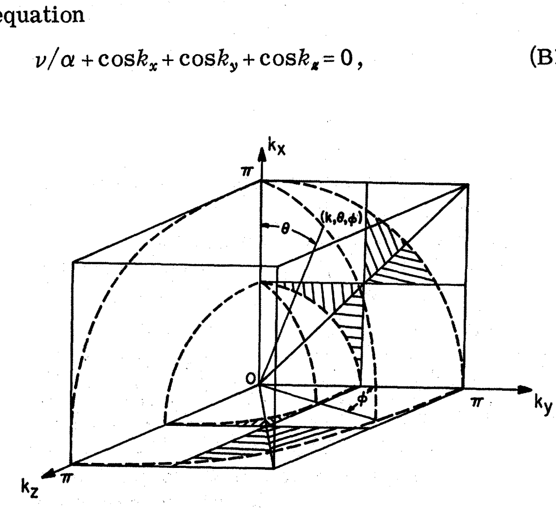

FIG. 5. An octant of the integration domain.

Thus, $\nu/\alpha = -3, -1, 1, 3$ are end-point singularities[10] of A_0 and A_0' corresponding to end points of contour of integration $(k_x, k_y, k_z) = (0, 0, 0)$, $(0, 0, \pi)$, $(0, \pi, \pi)$, (π, π, π), respectively. To see the nature of these singularities we consider, for simplicity,

$$D_0 = \frac{1}{\pi^3}\iiint_0^\pi \frac{dk_x\,dk_y\,dk_z}{\nu/\alpha + \cos k_x + \cos k_y + \cos k_z} ,$$

which has the same analytic properties as the A's. Since

$$\frac{1}{\pi^2}\iint_0^\pi \frac{dk_x\,dk_y}{\nu/\alpha + \cos k_x + \cos k_y + \cos k_z}$$

$$\sim C_1(a)\ln(\nu/\alpha + \cos k_z - a) + C_2(a) \qquad \text{(B2)}$$

for $\nu/\alpha + \cos k_z \sim a$, where $a = -2, 0, 2$, we observe that $D_0 \propto (\nu/\alpha - b)^{1/2}$ for $\nu/\alpha \sim b$, where $b = -3, -1, 1, 3$. Therefore the end-point singularities of A_0 and A_0' are all square-root branch points. It is well known that across the real axis between $\nu/\alpha = -3$ and 3, the imaginary parts of A_0 and A_0' change sign, while the real parts are continuous. So the branch cut lies on the real axis between -3 and 3, in the ν/α plane. Furthermore, there are two Riemann sheets for the part of the ν/α plane where $\mathrm{Re}(\nu/\alpha) < -1$.

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$$\cos(z\cos\phi) = J_0(z) + \sum_{n=1}^{\infty}(-1)^n J_{2n}(z)\cos 2n\phi$$

and obtain

$$M(k) = \int_0^1 d(\cos\theta)\, J_0(k\sin\theta)\cos(k\cos\theta)$$
$$= \int_0^1 x(1-x^2)^{-1/2}\cos[k(1-x^2)^{1/2}]\, J_0(kx)\, dx$$
$$= (\sin\sqrt{2}k)/\sqrt{2}k\ ;$$

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Cowley Theory of Long-Range Order in β-CuZn

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The Cowley theory is used to estimate the effect of nonstoichiometry on long-range order in β-CuZn alloys.

Accurate Ising-model calculations of the temperature dependence of long-range order in β-CuZn are available at the present only for the stoichiometric alloy.[1,2] To estimate the change in the long-range-order curve due to a departure from the stoichiometric composition, we have investigated the approximate theory of order developed[3] and revised[4] by Cowley. Although its thermodynamic formulation is not rigorous, we shall show that this theory does give a long-range-order curve for equiatomic β-CuZn in good agreement with Ising-model calculations except at the higher temperatures near T_c, and it can give the proper dependence on composition in the limit of low temperatures, so we suggest that it should give a reasonable estimate of the effect of nonstoichiometry over much of the range of temperature below T_c.

Cowley did not give an expression for long-range order in nonstoichiometric alloys in his papers. Our equations for the β-CuZn alloys are derived from his initial paper[3] after changing one approximation, which appears equivalent to using a simple form of the revised approach of his later papers.[4] Cowley developed an expression for the free energy in terms of the Warren short-range-order parameters α_l, which had been shown to have