Two-Magnon Bound States in a Ferromagnet

A. M. Bonnot and J. Hanus
Groupe de Physique des Etats Condensés, U.E.R. de Luminy, 70 Route Léon-Lachamp Marseille 9e, France
(Received 22 June 1972)

In this paper we show that in simple cubic (sc), bcc, and fcc ferromagnets with first-nearest-neighbor interactions there exists a region in the center of the Brillouin zone in which two-magnon bound states cannot exist, thus extending the known results for a sc lattice.

The existence, in an Heisenberg ferromagnet, of excitations of wave vector $\vec{K}$ corresponding to two units of spin deviation with an energy less than the added energies of two noninteracting spin waves of total momentum $\vec{K}$ has been demonstrated, at least in a simple cubic (sc) ferromagnet.[1,2] These bound states exist only when their momentum $\vec{K}$ is greater than $\vec{K}_0$, their energy is below the two-spin-wave continuum, and they have no width. These bound states and their observability have received quite some attention recently,[3,4] and Thorpe[5] claims that a weak repulsive force between magnons splits off a bound state above the continuum of a fcc ferromagnet at zero total momentum. He relates this state to the logarithmic divergency of the density of states at the top of the continuum. This result is quite surprising. The physical reason for the very existence of the bound state is an attraction between spin deviations; if a spin already deviates from its ground-state alignment, the energy required to create a second spin deviation is less for a neighboring spin that can be coupled to the former by the exchange interaction than if the two spins are outside the range of interaction. Actually the interactions between spin deviations are not always attractive. The effective interaction is strongly $\vec{K}$ dependent. Near the edges of the zone it is always attractive, but for small $\vec{K}$ it depends on the relative momenta.

In this paper we look at bound states with small momentum and show that they cannot exist for an isotropic-ferromagnetic exchange interaction irrespective of the crystal structure.

The analysis of the sc ferromagnet has been done analytically[1,2] in the [111] direction because this direction has such a degree of symmetry that $\cos\frac{1}{2}\vec{K}\cdot\vec{\Delta}$ is the same for all first neighbors $\vec{\Delta}$; in the bcc structure, the [100] direction has the same property, and we show that the states are very much the same. There is an excluded region around Γ, at the center of the Brillouin zone. It is not possible to evaluate simply the excluded region in the case of a fcc ferromagnet and perhaps it is not worth a numerical analysis.

To derive the conditions for the formation of bound states, we study the propagator for two spin waves at $T=0$ °K. The poles of the propagator give the excitation energies of the system. In terms of the unperturbed two-spin-waves propagator,

$$G_{\vec{K}}(\vec{L})=\frac{2JS}{N}\sum_{\vec{k}}\frac{e^{i\vec{k}\cdot\vec{L}}}{E-E(\frac{1}{2}\vec{K}+\vec{k})-E(\frac{1}{2}\vec{K}-\vec{k})}\,, \quad (1)$$

where the spin-wave energy is

$$E(\vec{k})=JS\sum_{\vec{\Delta}}(1-e^{i\vec{k}\cdot\vec{\Delta}}) \quad (2)$$

and the poles of the propagator are given by

$$\det[\delta(\vec{\Delta}-\vec{\Delta}')+A_{\vec{K}}(\vec{\Delta},\vec{\Delta}')]=0\,, \quad (3)$$

with

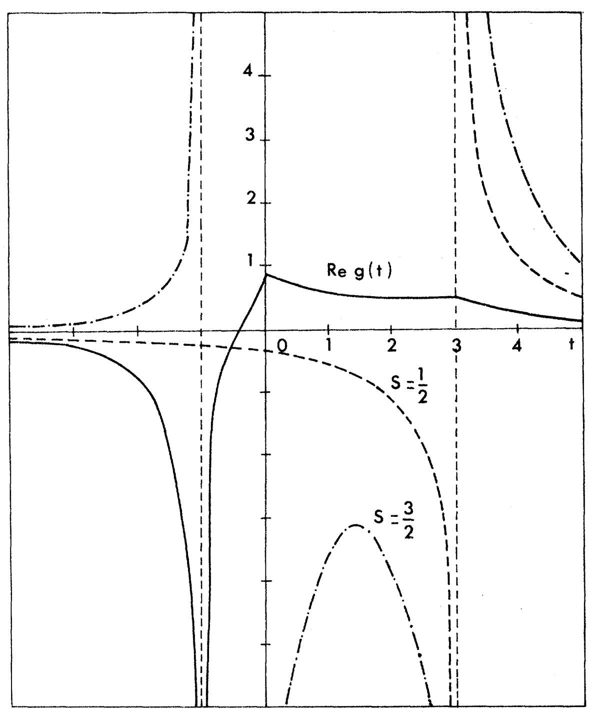

FIG. 1. Plot of the real part of the Green's function for a fcc lattice and of $6S-3+t/[t(t-3)]$ of Eq. (9) for $S=\frac{1}{2}$ and for $S>1$, as a function of $t=3-E/8JS$.

$$A_{\vec{K}}(\vec{\Delta}, \vec{\Delta}') = (1/2S)\left[\tfrac{1}{2}G_{\vec{K}}(\vec{\Delta} - \vec{\Delta}') + \tfrac{1}{2}G_{\vec{K}}(\vec{\Delta} + \vec{\Delta}') - \cos\tfrac{1}{2}\vec{K}\cdot\vec{\Delta}'\, G_{\vec{K}}(\vec{\Delta})\right] ,$$

where $\vec{\Delta}$ runs over the z nearest-neighbor sites, $\vec{K}$ is the momentum of the excitation, and the summation in $G_{\vec{K}}(\vec{L})$ is over the first Brillouin zone. Since two spin operators on different sites commute, $\sum_{\vec{\Delta}}$ can be replaced by $2\sum^{*}_{\vec{\Delta}}$, a summation over one-half the sites.

Equation (3) has been studied[1,2] in detail for the sc structure and is quite complicated for other structures. It is, nevertheless, easy to study it for $\vec{K}=0$. In this case we can classify the states according to the irreducible representations of Γ, the center of the Brillouin zone, and, in particular, the state of symmetry Γ_1 is given by

$$1 + \frac{2J}{N}\sum_{\vec{k}}\sum_{\vec{\Delta}}{}^{*}\, \frac{\cos\vec{k}\cdot\vec{\Delta}'(\cos\vec{k}\cdot\vec{\Delta} - 1)}{E(\Gamma_1) - 2E(\vec{k})} = 0 . \quad (4)$$

With Eqs. (1) and (2), we can reduce this expression to

$$1 - \frac{E}{4S^2 J}\, G_{\vec{K}=0}(\vec{\Delta}) = 0 . \quad (5)$$

The sign of $G(\vec{\Delta})$ is not obvious, and we express (5) in terms $G_{\vec{K}=0}(0)$: Better, to use published data, we introduce Watson's integrals[6]

$$g(t; p, q, r) = \frac{1}{\pi^3}\int\!\!\int_0^{\pi}\!\!\int dx\,dy\,dz\, \frac{\cos px \cos qy \cos rz}{t - \omega(x, y, z)} , \quad (6)$$

with $\omega(x, y, z)$, respectively, equal to $\cos x + \cos y + \cos z$, $\cos x \cos y \cos z$, and $\cos x \cos y + \cos y \cos z + \cos z \cos x$ for sc, bcc, and fcc lattices. Then

$$G_{\vec{K}}(0) = -(1/2u)g(t; 0, 0, 0) = -(1/2u)g(t) , \quad (7)$$

where $u = 1,\ 4,$ and 2;

$$t = 3 - E/4JS ,\quad 1 - E/16JS ,\quad 3 - E/8JS ,$$

for sc, bcc, and fcc lattices, respectively. The Γ_1 bound states are solutions of

$$1 - E/4S^2Jz + (E/8S^2Ju)(1 - E/2JSz)g(t) = 0 . \quad (8)$$

This equation never has any real solution for the cubic lattices; this was stated earlier[1,2] for the sc lattice. We will discuss it at greater length for the bcc lattice below. For a fcc lattice, Eq. (8) reads

$$g(t) + \frac{3(2S-1)+t}{(3-t)t} = 0 ,\quad t = 3 - \frac{E}{8JS} ; \quad (9)$$

the top of the continuum is given by $t \leqslant -1$, the bottom by $t \geqslant 3$, and $g(t)$ is sketched on Fig. 1.

For $-1 \leqslant t \leqslant 3$, we plot $\mathrm{Re}\,g(t)$ and we see that Eq. (8) has a root for $S=\frac{1}{2}$. It is conceivable that with some anisotropy[7] the virtual state can be pushed near the top of the band to give a resonance.[8]

For a fcc ferromagnet at Γ, there are two other

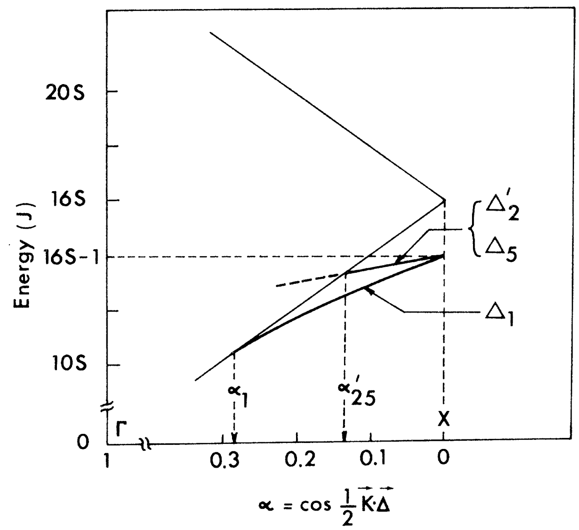

FIG. 2. Plot of the Δ bound-state bands in the [100] direction of the bcc Brillouin zone, near the X corner of the zone. $\alpha = \cos\frac{1}{2}\vec{K}\cdot\vec{\Delta}$ (for clarity we choose $S=\frac{1}{2}$ to calculate α_1, α'_{25}).

possible states Γ'_{25} and Γ_{12}, given by

$$g(t; 0, 0, 0) + 2g(t; 2, 0, 0) + g(t; 2, 2, 0) = 8S \quad \text{for}\ \Gamma'_{25} , \quad (10)$$

$$g(t; 0, 0, 0) + 2g(t; 2, 0, 0) - 2g(t; 1, 1, 0) + g(t; 2, 2, 0) - 2g(t; 1, 1, 2) = 8S \quad \text{for}\ \Gamma_{12} . \quad (11)$$

A simple analysis shows that they, also, have no real solution.[9]

The lattice's Green's functions for cubic lattices have been studied lately,[6,10] and we can take advantage of these results to find the excluded volume around the center of the Brillouin zone in which there is no real bound state. This is easily done if the propagator $G_{\vec{K}}(\vec{L})$ can be reduced to a one-spin-wave propagator: This can be achieved for the directions of the total momentum such that, in the energy of the two noninteracting spin waves,

$$E(\tfrac{1}{2}\vec{K} + \vec{k}) + E(\tfrac{1}{2}\vec{K} - \vec{k}) = 4JS\sum_{\Delta}^{*}(1 - \cos\tfrac{1}{2}\vec{K}\cdot\vec{\Delta}\cos\vec{k}\cdot\vec{\Delta}) . \quad (12)$$

$\cos\frac{1}{2}\vec{K}\cdot\vec{\Delta}$ has the same value for all neighboring sites $\vec{\Delta}$. In that way, the [111] direction was treated for the sc lattice; no such simplification occurs for the fcc lattice, but we give here more detailed results for a bcc lattice.

With $\vec{K}$ in the [100] direction, Eq. (12) reads

$$16JS - 4JS\alpha\sum_{\Delta}^{*}\cos\vec{k}\cdot\vec{\Delta} , \quad (13)$$

with $\alpha = \cos\frac{1}{2}\vec{K}\cdot\vec{\Delta}$. There are four possible roots of symmetry, Δ_1, Δ'_2, and doubly generate Δ_5, but for first-nearest-neighbor interaction, the degeneracy between Δ_5 and Δ_2' is not lifted and we have only two equations for the four roots. The Δ_1 state is given by

$$g(t;0,0,0)=\frac{(2S-1)\alpha+t}{t(t-\alpha)}, \qquad t=\frac{1}{\alpha}\left(1-\frac{E}{16JS}\right). \quad (14)$$

Below the continuum $t \geq 1$, the Δ_1 bound state will split off the continuum for $\alpha=\alpha_1$. Using published[10] values of $g(t=1;\, p,\, q,\, r)$, one finds $\alpha_1 = 0.393/(2S+0.393)$. At the X edge of the Brillouin zone, $\alpha=0$ and $E(X)=16JS-J$, which indicates that the state is located only on two sites.

The triply degenerate Δ_2', Δ_5 state is given by

$$t^2 g(t;0,0,0)-\tfrac{1}{2}g(t;\,2,0,0)-\tfrac{1}{2}g(2,2,0)=t+2S\alpha\ , \quad (15)$$

here again, when $\alpha \to 0$, $t\to\infty$, and $E=16SJ-J$. The bound-states band splits off below the continuum at α_{25}'. From Ref. 9 one gets $\alpha_{25}'=0.133/2S$, the resulting states are sketched on Fig. 2 for $S=\frac{1}{2}$.

We see from this short discussion that the results for the bcc and sc lattices are quite comparable; chances are that the situation is quite the same for the fcc lattice, although in that case it is not obvious how to evaluate the (large for sc and fcc lattices) excluded region around Γ.

With this absence of states around Γ, it is certain that the direct optical observation of two-magnon bound states in simple isotropic ferromagnet is ruled out. In presence of an anisotropic coupling,[7] the situation could be quite different, but to push a bound state above the continuum,[5] we need a repulsive mechanism. Perhaps, in EuS, the antiferromagnetic second-nearest-neighbor exchange interaction could provide such mechanism and explain the sharp structure observed on the magnon side bands.[11] The analysis of this point is outside the scope of this paper. In such a case, the divergence of the density of states at the top of the continuum will disappear.

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Spin-One Heisenberg Ferromagnet in the Presence of Biquadratic Exchange, M. Nauciel-Bloch, G. Sarma, and A. Castets [Phys. Rev. B 5, 4603 (1972)]. The receipt date of the manuscript, 21 October 1971, has not been mentioned. On p. 4605, column 2, line 16, the inequality should read $T_2 \lesssim T_0 < 2T_2$.

Sixth Moment of Dipolar-Broadened Magnetic-Resonance-Absorption Line Shapes in Crystals, E. T. Cheng and J. D. Memory [Phys. Rev. B 6, 1714 (1972)] and **Sixth Moment of the Magnetic Resonance Line Shape**, William F. Wurzbach and S. Gade [Phys. Rev. B 6, 1724 (1972)]. The expressions for the sixth moment of the magnetic-resonance line shape in these two papers are not consistent. In point of fact, neither is precisely correct. In the Cheng–Memory paper neglect of a factor of 2 in the heart of the calculation led to the neglect of several terms which should have been included in Eq. (3.15). When those are taken into account, several coefficients in Eq. (3.18) must be