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Two-spin-wave spectra of easy-plane ferromagnetic chains

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Abstract. The easy-plane ferromagnetic chain in an applied magnetic field is known to map onto a sine–Gordon field theory, in the classical continuum limit. The sine–Gordon field theory supports breather excitations which, when quantised, are identifiable as a hierarchy of bound states of several small-amplitude excitations. For increasing values of the interaction parameter, the highest members of the hierarchy become unstable to the emission of a soliton/anti-soliton pair. For a critical value of the interaction parameter, even the ground state of the quantised sine–Gordon field theory becomes unstable. For the quantum spin system, the excitations corresponding to the two lowest members of the hierarchy of breathers are the single-spin-wave and the two-spin-wave bound states. We examine the two-spin-wave bound-state excitations of the quantum spin system directly, using a large-S approach. Although our method does rely on large S, we recover previously derived results valid for arbitrary S, such as the exact two-spin-wave bound states for the isotropic Heisenberg ferromagnet and the expansion in the anisotropy about this result. In the limit of large anisotropy the two-spin-wave bound state becomes unstable, in a manner suggestive of the instability of the quantum sine–Gordon field theory.

1. Introduction

Mikeska [1] proposed that a one-dimensional easy-plane ferromagnet, when subjected to a symmetry-breaking magnetic field, can be mapped onto a one-dimensional sine–Gordon field theory. The angle φ representing the direction of the spins within the easy plane becomes the field of the sine–Gordon theory and the spin component perpendicular to the easy plane, S^z, is the canonically conjugate momentum field. The mapping between the spin system and the sine–Gordon system is restricted to occur in the classical continuum limit. This mapping is of considerable interest since it is well known that the sine–Gordon system supports very extraordinary types of elementary excitations [2]. There are the usual types of small-amplitude excitations which are spatially extended over the entire system. Since these excitations have small amplitudes, the effects of the non-linear interactions are small and may be taken into account by perturbation theory. These quasi-linear excitations are analogous to the spin waves in the spin system, which are well described by the harmonic approximation.

The other types of elementary excitations of the sine–Gordon system are more unusual. They have large amplitudes and only extend over a finite region of space. Unlike wave packets composed of the small-amplitude spin waves, these non-linear excitations do not disperse; that is, the non-linearity is such that these special excitations maintain their forms. These non-linear excitations may be uniformly translated over the entire system with a constant velocity. In the sine–Gordon system these excitations are characterised as soliton excitations or breather excitations. The soliton excitation consists of successive rotations between neighbouring spins, such that the spins rotate by 2π over a finite region of space. The breather excitations, on the other hand, consist of a field profile which has a uniform internal oscillation. The envelope of the field profile has an amplitude and a spatial extent which are determined by the frequency ω of the internal oscillation. The frequency is a continuous variable, which may take values in the range which extends from ω_0, the frequency associated with the gap in the spin-wave spectrum, all the way down to zero. The field profile for the breather solution can be written as

$$\varphi(z, t) = 4 \tan^{-1} \left(\frac{\surd(\omega_0^2 - \omega^2)}{\omega} \frac{\sin(\omega t)}{\cosh[\surd(\omega_0^2 - \omega^2) z/c]} \right) \tag{1.1}$$

where c is the characteristic velocity of the sine–Gordon field theory. The amplitude of the breather increases and its spatial extent decreases as the frequency ω approaches zero. The activation energy of the breather may be written as

$$E(\omega) = 2E_0(1 - \omega^2/\omega_0^2)^{1/2}$$

where E_0 is the rest energy of a soliton.

Clearly, the presence of an excitation spectrum with arbitrary low excitation energies presents problems to the statistical mechanics of the sine–Gordon field theory. Dashen *et al* [3] have performed a semi-classical quantisation of the breather excitations using the Bohr–Sommerfeld quantisation condition. The resulting breathers have the frequency of their internal oscillations quantised. Maki and Takayama [4] have demonstrated the equivalence between the hierarchy of the quantum breather excitations and the bound states formed between the spin waves. The hierarchy of breather excitations corresponds to the multi-spin-wave bound states according to the following prescription. The first-quantised breather corresponds to the single spin wave, which is expected on the basis of the classical breather profile becoming indistinguishable from that associated with the spin waves as ω approaches ω_0. The second-quantised breather corresponds to the bound state formed by two spin waves. This hierarchy is continued such that the nth-quantised breather corresponds the bound state formed by n spin waves. Thus, the breather spectrum now possesses a lower cut-off as well as an upper limit.

The mapping between the quantum spin system and the sine–Gordon system is quite suspect, since the zero-point motions of the spins do not distinguish sufficiently between the in-plane motions and the out-of-plane motions. Thus the quantum renormalisations are of a more isotropic nature than one might otherwise have suspected. Bishop [5] has suggested that as the temperature of the system is raised, the behaviour crosses over from that of the sine–Gordon model to that associated with the isotropic Heisenberg model in an applied field. The isotropic Heisenberg model is, like the sine–Gordon system, completely integrable in the continuum limit. The isotropic system has been shown to exhibit so called pulse solitons. Long and Bishop have noted the qualitative similarity between the pulse soliton and the breather excitations of both models. Fogedby [6] has used this similarity to suggest that the semi-classical quantised version of the pulse solitons also corresponds to multi-spin-wave bound states.

In this paper we shall take a first step toward exhibiting the relation between the breathers and the pulse solitons. That is, we shall examine the lowest-order non-trivial excitation of the hierarchy, the two-spin-wave bound states of the quantum spin system. The calculations we present here are complementary to the earlier work of Hood [7]. Hood's calculations are valid for arbitrary values of S, but are restricted to small values of D/J. Our work, on the other hand, is valid for arbitrary D/J but is limited to the case where $S \gg 1$. Nevertheless, our approach does produce results for the two-spin-wave bound-state dispersion relations which are very similar to those of Hood [7].

Our formulation does have the obvious advantage that it allows an immediate comparison between the isotropic Heisenberg limit and the easy-plane sine–Gordon limit. The surprising result of this work seems to be that the $q = 0$ two-spin-wave bound state bears more resemblance to the two-spin-wave bound states of the isotropic Heisenberg model, as studied by Wortis [8], than to the quantised breather excitations. This feature is caused by a subtle cancellation between the effects of the in-plane components of the Zeeman interaction with the out-of-plane components. This cancellation becomes more pronounced as the wavevector q approaches the boundary of the Brillouin zone. The energy of the zone-boundary two-spin-wave bound state is therefore identical to that of the corresponding two-spin-wave bound state of the isotropic Heisenberg spin system. The effect of the easy-plane anisotropy is channelled into the production of a second bound state of two spin waves. This second bound state may be resolved from the edge of the two-spin-wave continuum state for q values close to the zone boundary. In this paper we also examine the effect that the interactions have on the two-spin-wave continuum. In the harmonic-spin-wave approximation, the edge of the continuum shows a singularity. This singularity facilitates the production of the two-spin-wave bound states. However, the interactions which result in the formation of the two-spin-wave bound states also result in the washing-out of the divergence at the edge of the continuum.

The paper is organised as follows. In the next section we outline the harmonic spin-wave approximation and the two-spin-wave contributions to the dynamic spin–spin correlation functions. We then examine the effects that the anharmonic interactions have on the two-spin-wave states. We neglect all parts of the anharmonic interactions that do not couple to the states where two spin waves are simultaneously excited. That means we neglect the couplings which exist between the two-spin-wave sum processes and the two-spin-wave difference processes. This neglect may be justified at $T = 0$, where the two-spin-wave difference process will be absent, since it is only present due to thermal activation.

In § 4 we examine the various limits of the general result for the two-spin-wave spectrum derived in § 3. We show that our calculation reproduces the earlier results of Wortis [8] for the two-spin-wave bound states of the isotropic Heisenberg model. We also show that the first correction, in powers of D/J, to this isotropic limit reproduces the calculations of the two-spin-wave bound states which have been performed by Hood [7], valid for arbitrary S. In addition to the two-spin-wave bound states, we also examine the two-spin-wave continuum. We find that the two-spin-wave continuum contains a resonant branch as well as the scattering states. The effect of the interaction is also found to suppress the square-root singularity at the lower edge of the two-spin-wave continuum found in the harmonic theory. Our method is valid for arbitrary D/J, with $S \gg 1$, and can generate all the terms of the expansion in D/J. We shall show that when $D/J \sim S^2$, the x–y phase does become unstable to a singlet phase.

2. The two-spin-wave continuum

We first examine the two-spin-wave continuum in the harmonic-spin-wave approximation, and then in the next section we shall investigate the effect of the anharmonic interactions and the formation of the two-spin-wave bound state. The system under consideration is described by the Hamiltonian

$$\hat{H} = -\sum_i |J| \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - \sum_i D S_i^{z2} - \sum_i g\mu_B H^x S_i^x \tag{2.1}$$

where J is the strength of the isotropic ferromagnetic Heisenberg exchange interaction, D is the strength of the easy-plane anisotropy and H^x is the strength of the applied magnetic field which breaks the spin-rotational invariance of the easy plane. We shall denote $\sqrt{S(S+1)}$ by $\tilde{S}$ and, following the work of Riseborough [9], we describe the harmonic spin waves of the Hamiltonian by

$$\hat{H}_0 = \sum_k \{2J\tilde{S}[1-\cos(ka)] + g\mu_B H^x\}\frac{\tilde{S}}{2}\varphi_k\varphi_{-k} + \sum_k \{2J\tilde{S}[1-\cos(ka)] + 2D\tilde{S} + g\mu_B H^x\}(1/2\tilde{S})S_k^z S_{-k}^z. \tag{2.2}$$

This can be diagonalised, to lowest order in $1/S$, by expressing the canonically conjugate operators φ_k and S_k^z in terms of spin-wave creation and annihilation operations [10] through

$$\varphi_k = \alpha_k(a_k^+ + a_k)/\sqrt{2\tilde{S}} \tag{2.3a}$$

and

$$S_k^z = \mathrm{i}\beta_k\sqrt{\tilde{S}/2}\,(a_k^+ - a_k) \tag{2.3b}$$

where $\alpha_k = \beta_k^{-1}$ and is given by

$$\alpha_k^4 = \{2J\tilde{S}[1-\cos(ka)] + 2D\tilde{S} + g\mu_B H^x\}/\{2J\tilde{S}[1-\cos(ka)] + g\mu_B H^x\}. \tag{2.3c}$$

The resulting harmonic part of the spin-wave Hamiltonian is given by

$$\hat{H}_0 = \sum_k \omega_k a_k^+ a_k \tag{2.4a}$$

where the spin-wave dispersion relation is given by

$$\omega_k^2 = \{2J\tilde{S}[1-\cos(ka)] + 2D\tilde{S} + g\mu_B H^x\}\{2J\tilde{S}[1+\cos(ka)] + g\mu_B H^x\}. \tag{2.4b}$$

The two-spin-wave continuum excitations show up directly in the x–x component of the dynamic spin correlation function [9]. The contribution due to the excitation of the two-spin-wave continuum can be written as

$$\tfrac{1}{8}\sum_k (\alpha_{q/2-k}^2\alpha_{q/2+k}^2 + \beta_{q/2-k}^2\beta_{q/2+k}^2 - 2)(1 + N(\omega_{q/2-k}))(1 + N(\omega_{q/2+k})) \times \delta(\omega - \omega_{q/2-k} - \omega_{q/2+k}). \tag{2.5}$$

This represents the simultaneous creation of two spin waves with energy ω and total wavevector q. The allowed range of energies, for fixed q, approximately lies within the range

$$2\omega_{q/2} < \omega < \omega_{q/2-\pi} + \omega_{q/2+\pi}. \tag{2.6}$$

The width of the spin-wave continuum is narrowest for values of q near $q = \pi$.

The two-spin-wave continuum, calculated in the harmonic approximation, exhibits square-root singularities at its upper and lower boundaries. This can be seen by performing the summation over k in the above expression, and utilising the properties of the dirac delta function. This results in the expression

$$\tfrac{1}{8}(\alpha^2_{q/2-k}\alpha^2_{q/2+k} + \beta^2_{q/2-k}\beta^2_{q/2+k} - 2)(1 + N(\omega_{q/2-k})) \times (1 + N(\omega_{q/2+k}))/|\partial(\omega_{q/2-k} - \omega_{q/2+k})/\partial k| \tag{2.7}$$

in which k has the value given by the solution of $\omega = \omega_{q/2+k} + \omega_{q/2+k}$. At the extremities of the two-spin-wave continuum, the total energy $\omega_{q/2+k} + \omega_{q/2+k}$ is an extremum, and therefore the denominator vanishes. At the lower edge of the continuum, the numerator simplifies to

$$\tfrac{1}{2}[D\tilde{S}(1 + N(\omega_{q/2}))/\omega_{q/2}]^2. \tag{2.8}$$

This shows that the two-spin-wave continuum has a square-root singularity at the edges, and that the strength of the singularity is a signature of the easy-plane character of the system [9, 11].

Steiner *et al* [12] have recently reported the observation of structure associated with the lower edge of the two-spin-wave continuum in inelastic neutron scattering experiments. Both the excitation energy and the spectral intensity are in reasonable agreement with those predicted by the harmonic-spin-wave theory.

In the next section we shall obtain a general expression for the two-spin-wave spectrum when anharmonic interactions are included. The anharmonic interactions will be treated within the random phase approximation.

3. The effects of the interactions

The lowest-order terms of the anharmonic interactions are rewritten in the appendix, such that the pairing terms appear as the sum of separable interactions. That is, the anharmomic interactions are written as

$$\hat{H}_{\text{int}} = -\frac{1}{4\tilde{S}}\sum_{i=1}^{8}\sum_{k,k',q} \Lambda_q^{(i)} M^{(i)}_{k,q} M^{(i)}_{k',q} a^+_{q/2-k} a^+_{q/2+k} a_{q/2+k'} a_{q/2-k'}, \tag{3.1}$$

where the matrix elements are given in the appendix. It should be noted that we have neglected the terms which produce the coupling between the two-spin-wave sum and difference spectra. This neglect is justified at $T = 0$ where, as we have shown, the zeroth-order two-spin-wave difference process vanishes.

We shall define a two-spin-wave propagator by specifying the matrix elements

$$\Pi_{k,k'}(q,t)^{(i,\ j)} = -\mathrm{i}\theta(t) M^{(i)}_{k,q} M^{(j)}_{k',q} \langle a_{q/2-k}(t) a_{q/2+k}(t) a^+_{q/2+k'}(0) a^+_{q/2-k'}(0)\rangle. \tag{3.2}$$

The equation of motion for this two-spin-wave propagator is found to be

$$\mathrm{i}(\partial/\partial t)\Pi_{k,k'}(q,t)^{(i,j)} = M^{(i)}_{k,q} M^{(j)}_{k',q} (\delta(t)\langle a_{q/2-k} a_{q/2+k} a^+_{q/2+k'} a^+_{q/2-k'}\rangle - \mathrm{i}\theta(t)\langle [a_{q/2-k} t) a_{q/2+k}(t); \hat{H}(t)]_- a^+_{q/2+k'}(0) a^+_{q/2-k'}(0)\rangle). \tag{3.3}$$

The Hamiltonian is then written as the sum of the quadratic term and the pairing interaction. The above equation then simplifies to the form

$$[\mathrm{i}(\partial/\partial t) - \omega_{q/2-k} - \omega_{q/2+k}]\Pi_{k,k'}(q,t)^{(i,j)} = \delta(t)[\delta(k-k') + \delta(k+k')] M^{(i)}_{k,q} M^{(j)}_{k',q} - \mathrm{i}\theta(t) M^{(i)}_{k,q} M^{(j)}_{k',q} \langle [a_{q/2-k}(t) a_{q/2+k}(t); \hat{H}_{\text{int}}(t)]_- a^+_{q/2+k'}(0) a^+_{q/2-k'}(0)\rangle. \tag{3.4}$$

The commutator with the interaction leads to higher-order correlation functions. We shall decouple the resulting hierarchy of equations of motion, by making the replacements

$$\delta(q/2 + k_1 - q/2 - k)\langle a^{+}_{q'2-k_1}(t)a_{q/2-k}(t)a_{q'/2+k_2}(t)a_{q'/2-l_2}(t)a^{+}_{q/2-k'}(0)a^{+}_{q/2+k'}(0)\rangle \to 0$$

$$\delta(q'/2 + k_1 - q/2 + k)\langle a^{+}_{q/2-k_1}(t)a_{q/2+k}(t)a_{q'/2+k_2}(t)a_{q'/2-k_2}(t)a^{+}_{q/2-k'}(0)a^{+}_{q/2+k'}(0)\rangle \to 0$$

$$\delta(q'/2 - k_1 - q/2 - k)\langle a_{q/2-k}(t)a^{+}_{q'/2+k_1}(t)a_{q'/2+k_2}(t)a_{q'/2-k_2}(t)a^{+}_{q/2-k'}(0)a^{+}_{q/2+k'}(0)\rangle \to \delta(q - q')\delta(k + k_1)\langle a_{q/2+k_2}(t)a_{q/2-k_2}(t)a^{+}_{q/2-k'}(0)a^{+}_{q/2+k'}(0)\rangle$$

and

$$\delta(q'/2 - k_1 - q/2 + k)\langle a_{q/2+k}(t)a^{+}_{q'/2+k_1}(t)a_{q'/2+k_2}(t)a_{q'/2-k_2}(t)a^{+}_{q/2-k'}(0)a^{+}_{q/2+k'}(0)\rangle \to \delta(q - q')\delta(k - k_1)\langle a_{q/2+k_2}(t)a_{q/2-k_2}(t)a^{+}_{q/2-k'}(0)a^{+}_{q/2+k'}(0)\rangle \quad (3.5)$$

We have neglected the contractions that occur entirely between the operators associate with the interaction. Those terms contribute to the one-loop renormalisation of the spin-wave energies [13, 14]. Therefore, those terms can be absorbed into a renormalisation of the spin-wave energies appearing on the left-hand side of equation (3.4).

This decoupling procedure is similar to that used by Tognetti *et al* [15]; however, as previously mentioned, we neglect correlations between excitations other than the two-spin-wave sum processes. Thus the neglect of the coupling between the two-spin-wave sum and difference processes restricts the validity of our calculation to $T = 0$.

The Fourier transform of the two-spin-wave propagator is defined by

$$\Pi_{kk'}(q, \omega)^{(i,j)} = \int_{-\infty}^{\infty} \exp(\mathrm{i}\omega t)\Pi_{k,k'}(q, t)\, \mathrm{d}t. \quad (3.6)$$

On Fourier transforming the equation of motion, we obtain a closed set of coupled equations:

$$(\omega - \omega_{q/2-k} - \omega_{q/2+k})\Pi_{k,k'}(q, \omega)^{(i,j)} = [\delta(k - k') + \delta(k + k')]\, M^{(i)}_{k,q}M^{(j)}_{k',q} - \sum_{j'=1}^{8} \frac{\Lambda^{(j')}_q}{4\tilde{S}} M^{(i)}_{k,q)}(M^{(j')}_{k,q} + M^{(j')}_{-k,q}) \sum_{k_2} \Pi_{k_2,k'}(q, \omega)^{(j',j)}. \quad (3.7)$$

On rearranging these equations and then summing over k, we find that

$$\sum_k \Pi_{k,k'}(q, \omega)^{(i,j)}$$

satisfies the matrix equation

$$\sum_{j'} D(q, \omega)^{(i,j')} \sum_k \Pi_{k,k'}(q, \omega)^{(j,',j)} = \sum_k \Pi^0_{k,k'}(q, \omega)^{(i,j)} \quad (3.8)$$

where

$$D(q, \omega) = \delta_{i,j} + \frac{\Lambda^{(j)}_q}{8\tilde{S}} \sum_k \frac{(M^{(i)}_{k,q} + M^{(i)}_{-k,q})(M^{(j)}_{k,q} + M^{(j)}_{-k,q})}{\omega - \omega_{q/2-k} - \omega_{q/2+k}} \quad (3.9a)$$

and

$$\sum_k \Pi^{(0)}_{k,k'}(q,\omega)^{(i,j)} = \frac{(M^{(i)}_{k',q} + M^{(i)}_{-k',q})M^{(j)}_{k',q}}{\omega - \omega_{q/2-k'} - \omega_{q/2+k'}}. \tag{3.9b}$$

Inversion of the above matrix equation gives the general expression for the matrix

$$\sum_k \Pi_{k,k'}(q,\omega)^{(i,j)}.$$

The quantity of physical importance is

$$\mathrm{Im}\left(\sum_{k,k'} \Pi_{k,k'}(q,\omega)^{(1,1)}\right)$$

since this is the part of the two-spin-wave propagator which appears in the spin–spin correlation function.

In the next section we shall examine various limits of the result contained in equation (3.8).

4. Results and discussion

The two-spin-wave continuum contribution to the $T = 0$, x–x component of the spin–spin correlation function is given by the imaginary part of $\pi(q,\omega)^{(1,1)}$. At absolute zero, the two-spin-wave difference process does not contribute. In addition to the two-spin-wave continuum, there are also the two-spin-wave bound states. These bound states occur in the regions where the delta functions,

$$\delta(\omega - \omega_{q/2-k} - \omega_{q/2+k}),$$

occurring in the imaginary part of $\Pi(q,\omega)$ are identically zero. In these regions, the only contributions to the spectral density are the values of ω and q where the determinant of the matrix $D(q,\omega)$ vanishes. We shall examine the limiting case in which the strength of the easy-plane anisotropy D is zero, as well as the modifications that occur when one tries to expand around the $D = 0$ limit. Then we shall examine the limit of large D/J.

4.1. The isotropic limit

In the limit of vanishing single-ion anisotropy, the spectrum associated with the two-spin-wave bound states can be written as the solution of a simple polynomial equation. This simplification occurs due to the fact that in this limit, the matrix elements of $D(q,\omega)$ can be evaluated analytically. The energy denominator occurring in $D(q,\omega)$ can be written as

$$\omega - \omega_{q/2-k} - \omega_{q/2+k} = (\omega - 2g\mu_B H^x - 4J\tilde{S}) + 4J\tilde{S}\cos(qa/2)\cos(ka). \tag{4.1}$$

The summations over k in the expression for $D(q,\omega)$ can be performed by relating them to the summation

$$\sum_k [(\omega - 2g\mu_B H^x - 4J\tilde{S}) + 4J\tilde{S}\cos(qa/2)\cos(ka)]^{-1}$$
$$= \pm\{(\omega - 2g\mu_B H^x - 4J\tilde{S})^2 - [4J\tilde{S}\cos(qa/2)]^2\}^{-1/2}. \tag{4.2}$$

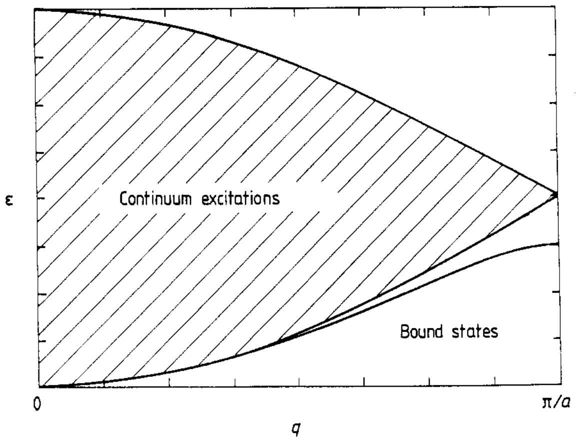

Figure 1. The dispersion energy against momentum for the $T = 0$ two-spin-wave spectrum for the isotropic Heisenberg ferromagnet. In addition to the continuum, there exists a continuous branch of bound states.

The zeros of the determinant of $D\ (q, \omega)$ locate the energies of the two-spin-wave bound states. In the isotropic limit, the determinant can be written as the determinant of a 2×2 matrix. The resulting equation for the energies of the two-spin-wave bound states is

$$1 = (1/2\tilde{S})[1 - 1/8\tilde{S} + x/\cos(qa/2)][1 \pm x/\surd(x^2 - 1)] \tag{4.3a}$$

where

$$x = (\omega - 2q\mu_B H^x - 4J\tilde{S})/4J\tilde{S}\cos(qa/2). \tag{4.3b}$$

This can be reduced to a cubic equation. Of the three roots, only one corresponds to a spin-wave-bound state of the above equation. The other solutions either do not satisfy the original equation or they lay within the continuum of two-spin-wave scattering states.

In addition to the two-spin-wave bound states, we find that there is a resonance within the continuum of two-spin-wave states. This is in agreement with the work of Haldane [16, 17], which suggests that for $S > \frac{1}{2}$ there should be two distinct branches in the two-spin-wave spectrum, which may be composed of either resonant or bound states. The resonance lies in the upper half of the continuum close to the upper edge of the continuum. As we shall show later, the introduction of easy-plane anisotropy has the effect of distorting the spin-wave resonance, pulling the resonance outside the lower edge of the continuum for q close to π/a such that the resonance and the anisotropic-induced bound state still form one continuous branch. On excluding terms of order $1/S^2$, this equation becomes identical to that previously derived by Wortis [8] for the two-spin-wave bound states of the isotropic Heinsenberg ferromagnet. Since the equation derived by Wortis is exact at zero temperature, we see that the above procedure reproduces the exact equation up to order $1/S^2$. However, the terms of order $1/S^2$ and higher in the above equation are spurious and must cancel with the terms of the corresponding order that we have neglected in arriving at our result (such as the terms which normalise the spin-wave energies and similar terms that renormalise the two-spin-wave interactions [18]). In figure 1 we depict the spectrum of the two-spin-wave continuum and the two-spin-wave bound states as derived from the exact equation, with $S = 1$.

The leading corrections to the isotropic Heinsenberg limit may be obtained by expanding the determinant in powers of D/J. It is instructive to examine the first-order corrections since these lead to the formation of another type of two-spin-bound state that exists for q values close to the Brillouin-zone boundary. This bound state has been previously found by Hood [7]. We shall see that our analysis reproduces the earlier work of Hood, when we expand the determinant and keep only the lowest powers of D/J.

4.2. *Limit of small easy-plane anisotropy*

The lowest order in the $1/S$ contribution to the determinant is given by the expression

$$1+\frac{1}{2\tilde{S}}\frac{g\mu_B H^x}{4}\sum_k\frac{[(\alpha^2_{q/2-k}+\beta^2_{q/2-k})(\alpha^2_{q/2+k}+\beta^2_{q/2+k})-4\beta^2_{q/2-k}\beta^2_{q/2+k}]}{(\omega-\omega_{q/2-k}-\omega_{q/2+k})}$$
$$+\frac{1}{2\tilde{S}}J\tilde{S}\frac{[\cos^2(qa/2)+\cos^2(ka)-2]\beta^2_{q/2-k}\beta^2_{q/2+k}}{(\omega-\omega_{q/2-k}-\omega_{q/2+k})}$$
$$+\frac{1}{2\tilde{S}}J\tilde{S}\sum_k\frac{[\cos^2(qa/2)+\cos^2(ka)-2\cos(qa/2)\cos(ka)]\alpha^2_{q/2-k}\alpha^2_{q/2+k}}{(\omega-\omega_{q/2-k}-\omega_{q/2+k})}$$
$$+\frac{1}{2\tilde{S}}J\tilde{S}\sum_k\frac{[\cos^2(ka)-\cos^2(qa/2)]2}{(\omega-\omega_{q/2-k}-\omega_{q/2+k})}$$
$$+\frac{1}{2\tilde{S}}J\tilde{S}\sum_k\frac{[1-\cos(q/2+k)a]\beta^2_{q/2-k}\alpha^2_{q/2+k}}{(\omega-\omega_{q/2-k}-\omega_{q/2+k})}$$
$$+\frac{1}{2\tilde{S}}J\tilde{S}\sum_k\frac{[1-\cos((q/2-k)a)]\alpha^2_{q/2-k}\beta^2_{q/2+k}}{(\omega-\omega_{q/2-k}-\omega_{q/2+k})}. \qquad (4.4)$$

These terms dominate the determinant for most q values, and give rise to the production of the two-spin-wave bound state which continues onto the two-spin-wave bound state of the isotropic Heisenberg limit, as D tends to zero. That is, the above form reproduces the lowest-order terms in $1/\tilde{S}$ of equation (4.3), when both α and β tend to unity. The above expression, when expanded to order D/J both in the numerators and the denominators, results in the expression

$$1-\frac{1}{2\tilde{S}}\left\{1+\left[\frac{x}{\cos(qa/2)}\right]\right\}[1\pm x/\surd(x^2-1)]\mp(1/\tilde{S})[D/4J\tilde{S}\cos(qa/2)](x^2-1)^{-1/2} \qquad (4.5a)$$

in which x is given by

$$x=(\omega-2g\mu_B H^x-2D\tilde{S}-4J\tilde{S})/4J\tilde{S}\cos(qa/2). \qquad (4.5b)$$

The above expression coincides with the terms of order $1/S$ previously derived by Hood [7].

The next terms in the expansion of the determinant are of order $1/\tilde{S}^2$. There are two types of such terms. One type represents small modifications of lower-order terms. These are spurious and may be eliminated by renormalising the interactions between the spin-waves. We have ignored such renormalisations, in both the spin-wave energies and the interactions. The second types of term are of greater importance, since they give rise to a change of sign in the determinant as ω approaches the bottom of the

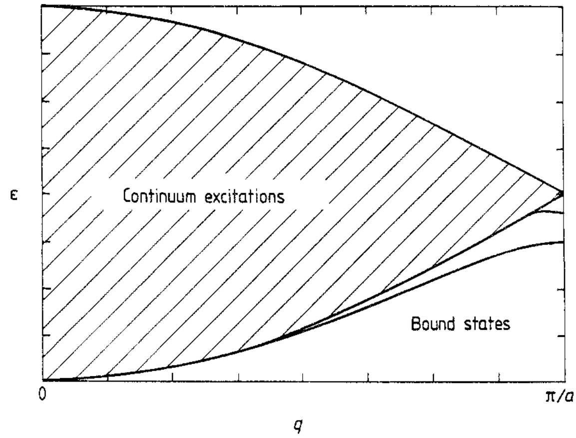

Figure 2. The two-spin-wave dispersion for the $T = 0$ Heisenberg ferromagnet with small single-site anisotropy. The anisotropy deforms the resonance in the continuum until it emerges as a second bound state, for q close to π/a.

two-spin-wave continuum. That is, they give rise to a second type of two-spin-wave bound state. This latter term can be written as

$$-[D/8J\tilde{S}^2\cos^2(qa/2)][1 \pm x/\surd(x^2-1)] \tag{4.6}$$

for $g\mu_B H^x > 2D\tilde{S}$. This agrees with a similar term found by Hood.

As previously noted, the effect of the anisotropy is to lower the energy of the two-spin-wave resonance, so it emerges from the continuum as a true bound state. Clearly, this analysis is based on an approximation which neglects higher powers of $1/\tilde{S}$ and cannot be continued down to $S = 1/2$, since for $S = 1/2$ the local anisotropy is diagonal and for $S = 1/2$ one-dimensional spin systems can only support one branch and two-spin-wave bound states or resonances [16, 17].

We note that the spurious terms of order $1/\tilde{S}^2$ have a negligible effect on the formation of the two-spin-wave bound states. For example, the single-ion bound state splits off from the bottom of the continuum when

$$\cos(qa/2) = D/(4J\tilde{S}) + O(D/J)^2$$

and is independent of S, to leading order in D/J. This can also be seen by examining the point $q = \pi/a$. The two-spin-wave bound state

$$|\psi_1\rangle = \sum_i \exp(i\pi R_i/a) a_i^+ a_i^+ \, |0\rangle \tag{4.7a}$$

has energy

$$E_1 = 4J\tilde{S} + 2D\tilde{S} + 2g\mu_B H^x - D \tag{4.7b}$$

while the other 'exchange' bound state

$$|\psi\rangle = \sum_i \exp[i\pi(R_i/a + 1/2)] a_i^+ a_{i+1}^+ \, |0\rangle \tag{4.8a}$$

with energy

$$E_2 = 4J\tilde{S} + 2D\tilde{S} + 2g\mu_B H^x - J. \tag{4.8b}$$

These states and the binding energies are precisely those found by Hood, and are completely unaffected by the spurious terms.

In figure 2 we show the two-spin-wave continuum and the two-spin-wave bound states, as determined by retaining terms in the determinant up to order D/J only. The bound state due to the single-ion anisotropy may be resolved from the edge of the two-spin-wave continuum for values of q close to the boundary of the Brillouin zone. We have taken the value of $D/J = 9/23.6$. The dispersion associated with this bound state is of order $D^2/2J$ and is thus negligible, without our approximation. However, continuity with the two-spin-wave resonance does strongly suggest that the sign associated with the dispersion is correct, and that the entire branch can be described by

$$\omega \simeq 4J\tilde{S} + 2g\mu_B H^x + D(2\tilde{S} - 1) + 4J\tilde{S}(2\tilde{S} - 1)\cos^2(qa/2)[1 - (2\tilde{S} + 1)\cos^2(qa/2)]$$

for $\cos(q/2) \simeq 0$. For larger values of $\cos(q/2)$, the resonance has a position close to that of the isotropic Heisenberg system.

In addition to introducing a resonance in the two-spin-wave continuum, the interactions also suppress the square-root singularity at its lower edge. In the harmonic theory, to lowest order in D/J, the spectrum near $x \simeq 1$ is given by

$$[1/8J\tilde{S}\cos(qa/2)][1/\surd(1 - x^2)](D/J)^2[1 + g\mu_B H^x/2J\tilde{S} - \cos(qa/2)]^{-2}.$$

The effect of the interactions is to replace this singularity by a spectral density which, to leading order in S, approaches zero at the lower edge as

$$[\tilde{S}\cos(qa/2)/J](D/J)^2\sqrt{1 - x^2}[1 + g\mu_B H^x/2J\tilde{S} - \cos(qa/2)]^{-2} \times [1 + D/J - \cos(qa/2)]^{-2}.$$

This expansion in D/J can be pursued to higher order; however, the series is poorly convergent when the parameter $D/\sqrt{HJ}$ becomes too large. Under such circumstances the determinants must be handled numerically. In the next section, we shall investigate the limiting form that is obtained when $D/J \gg 1$.

4.3. *The large-anisotropy limit*

For large anisotropy, $D/J \gg 1$, and a fixed value of the spin one expects that the x–y phase will become unstable to a singlet phase, in which the excitations are dominated by the value of the easy-plane anisotropy. For example, for $S = 1$ and $D/J \gg 1$, one may evaluate the spin-wave spectrum by decoupling the equations of motion, to obtain

$$\omega_k^2 = D(D - 4J\cos(ka)) \tag{4.9}$$

to leading order in J. This represents small-amplitude excitations away from the $S^z = 0$ ground state. However, the spin-wave dispersion (2.4*b*) derived previously shows no evidence of such an instability. We shall, therefore, examine the two-spin-wave bound states in this regime in order to determine the mechanism whereby the x–y phase becomes instable.

When the easy-plane anisotropy is sufficiently large, $D/J \gg 1$, the fluctuations of the spins are mainly confined to lie within the easy plane as can be seen by comparing the form factors $|\alpha_k|$ and $|\beta_k|$. Thus, in the limit of large anisotropy, the dominant part of the determinental equation reduces to

$$0 = 1 + \frac{1}{2\tilde{S}}\frac{g\mu_B H^x}{4}\sum_k \frac{\alpha^2_{q/2-k}\alpha^2_{q/2+k}}{\omega - \omega_{q/2-k} - \omega_{q/2+k}} + \frac{1}{2\tilde{S}}J\tilde{S}$$
$$\times \sum_k \frac{[\cos(qa/2) - \cos(ka)]^2 \alpha^2_{q/2-k}\alpha^2_{q/21k}}{\omega - \omega_{q/2-k} - \omega_{q/2+k}} + \frac{g\mu_B H^x J\tilde{S}}{16\tilde{S}^2}$$
$$\times \sum_{kk'} \frac{\alpha^2_{q/2-k}\alpha^2_{q/2+k}(\cos^2 \mathrm{k} - \cos k \cos k')}{\omega - \omega_{q/2-k} - \omega_{q/2} + k}\,\frac{\alpha^2_{q/2-k'}\alpha^2_{q/2+k'}}{\omega - \omega_{q/2-k'} - \omega_{q/2+k'}}. \tag{4.10}$$

Equation (4.10) simplies in the limit $H^x \to 0$, where

$$\pi\tilde{S}\sqrt{\frac{2J}{D}} - 1 = \frac{x}{4}\frac{1 + (qa/\pi) - 1)\cos(qa/2)}{\sin(qa/2)} - \tfrac{1}{2}\frac{1-x^2}{\sqrt{[1 - x^2\sin^2(qa/4)]}}\frac{\sin^2(qa/2)}{\cos(qa/2)}$$
$$\times \ln\left|\frac{\tan(qa/8 + \pi/4) + \sqrt{\{[1 + x\sin(qa/4)]/[1 - x\sin(qa/4)]\}}}{\tan(qa/8 - \pi/4) - \sqrt{[\{1 + x\sin(qa/4)]/[1 - x\sin(qa/4)]\}}}\right|$$
$$- \tfrac{1}{2}\frac{1-x^2}{\sqrt{[1 - x^2\cos^2(qa/4)]}}\frac{\cos^2(qa/2)}{\sin(qa/2)}$$
$$\times \ln\left|\frac{\tan(qa/8) + \sqrt{\{[1 + x\cos(qa/4)/[1 - x\cos(qa/4)]\}}}{\tan(qa/8) - \sqrt{\{[1 + x\cos(qa/4)]/[1 - x\cos(qa/4)]\}}}\right| \tag{4.11}$$

where $x = \omega/[2\tilde{S}\sqrt{2JD}\sin(ga/2)]$.

For the values of $\sqrt{2D/J}/16\tilde{S} < (\pi/16)/(1 + \pi/4)$, this equation does not possess a solution. Thus, as $H^x \to 0$, both bound states become degenerate with the bottom of the continuum.

For $\sqrt{2D/J}/16\tilde{S} > (\pi/16)/(1 + \pi/4)$, a bound state splits off from the continuum at $q = \pi/a$ and for larger values of this parameter, the branch extends to lower values of q, until

$$(1/16\tilde{S})\sqrt{2D/J} = \pi/24,$$

when it reaches $q = 0$. On further increasing the coupling strength to the value

$$(1/16\tilde{S})\sqrt{2D/J} = \pi/8,$$

one finds that our approximation for the two-spin-wave bound state becomes soft at $q = 0$, signalling the proximity to an instability of the ground state due to the emission of $q = 0$ bound-spin-wave pairs. Although this instability may be spurious, since our technique is only expected to produce reasonable results when

$$(1/16\tilde{S})\sqrt{2D/J} \ll 1,$$

such an instability may be expected to occur to a singlet state [16].

Although for reasonable values of the coupling strength there is no solution of equation (4.9), $H^x = 0$, this conclusion immediately changes on application of an infinitesimally small field. In the limit $q = 0$ and $g\mu_B H^x/2J\tilde{S} \ll 1$ one finds that there is only one two-spin-wave bound state. Its energy is given by

$$\omega = 2\omega_0[1 - \tfrac{1}{2}(\sqrt{2D/J}/16\tilde{S})^2(1 - \sqrt{2D/J}/16\tilde{S} + \ldots)] \tag{4.12}$$

where the coupling strength $\sqrt{2D/J}/16\tilde{S} < 1$. This coupling constant is the same as that previously identified by Mikeska and Patzak [14]. To lowest order in the coupling constant, equation (4.11) agrees with the second breather of the quantum sine–Gordon theory [3, 4].

5. Summary

We have examined the two-spin-wave states of an easy-plane ferromagnet. The spectrum consists of a continuum of two-spin-wave scattering states and two branches of two-spin-wave bound states. The bound-state branch of higher energy merges with the continuum for wavevectors close to the zone boundary and then continues its existence for smaller q as a resonance near the top edge of the two-spin-wave continuum. The effect of the bound state is to reduce the square-root singularity at the lower edge of the two-spin-wave continuum.

A surprising result is that for q close to zero, the two-spin,wave bound states and resonant branches do retain the characteristics of the isotropic Heisenberg ferromagnet, until $D \sim \sqrt{HJ}$. For larger values of D/J, the isotropic or x–y phase becomes unstable by emission of bound pairs of spin waves.

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Appendix. Anharmonic interactions

The anharmonic interactions can be separated into two distinct classes: local interactions stemming from the Zeeman energy, and non-local interactions due to the Heisenberg exchange interaction. The lowest-order anharmonic interactions are tabulated in reference [13]. We shall rewrite the pairing part of these interactions as the sum of separable interactions:

$$\hat{H}_{\text{int}} = -\frac{1}{4\tilde{S}}\sum_{i=1}^{8}\sum_{k,k',q} \Lambda_q^{(i)} M_{k,q}^{(i)} M_{k',q}^{(i)} a^+_{q/2-k} a^+_{q/2+k} a_{q/2+k'} a_{q/2-k'} \tag{A1}$$

in which the total wavevector is conserved modulo $2\pi/a$. The matrix elements characterising the vertices are given by

$$\Lambda_q^{(1)} = \Lambda_q^{(2)} = g\mu_B H^x$$

$$M_{k,q}^{(1)} = \tfrac{1}{2}(\alpha_{q/2-k}\alpha_{q/2+k} - \beta_{q/2-k}\beta_{q/2+k})$$

$$M_{k,q}^{(2)} = \tfrac{1}{2}(\beta_{q/2-k}\alpha_{q/2+k} + \alpha_{q/2-k}\beta_{q/2+k})$$

$$\Lambda_q^{(3)} = -4g\mu_B H^x + 2J\tilde{S}[2\cos^2(qa/2) - \cos(qa/2) - 4]$$

$$M_{k,q}^{(3)} = \tfrac{1}{2}(\beta_{q/2-k}\beta_{q/2+k})$$

$$\Lambda_q^{(4)} = J\tilde{S}[1 - 2\cos(qa/2)]$$

$$M^{(4)}_{k,q} = 2\alpha_{q/2-k}\alpha_{q/2+k}\sin[(q2-k)a/2]\sin[(q/2+k)a/2]$$
$$\Lambda^{(5)}_q = +J\tilde{S}\,2\cos(qa/2)$$
$$M^{(5)}_{k,q} = \tfrac{1}{2}\{4\alpha_{q/2-k}\alpha_{q/2+k}\sin[(q/2-k)a/2]\sin[(q/2+k)a/2] + \beta_{q/2-k}\beta_{q/2+k}\}$$
$$\Lambda^{(6)}_q = 4J\tilde{S}$$
$$M_{k,q} = \tfrac{1}{2}[\beta_{q/2-k}\beta_{q/2+k}\cos(ka)]$$
$$\Lambda^{(7)}_q = \Lambda^{(8)}_q = 2J\tilde{S}$$
$$M^{(7)}_{k,q} = \tfrac{1}{2}\{2\beta_{q/2-k}\alpha_{q/2+k}\sin[(q/2+k)a/2]\cos(ka/2) + 2\beta_{q/2+k}\alpha_{q/2-k}\sin[(q/2-k)a/2]\cos(ka/2)\}$$
$$M^{(8)}_{k,q} = \tfrac{1}{2}\{2\beta_{q/2-k}\alpha_{q/2+k}\sin[(q/2+k)a/2]\sin(ka/2) - 2\beta_{q/2+k}\alpha_{q/2-k}\sin[(q/2-k)a/2]\sin(ka/2)\}. \qquad \text{(A2)}$$

In the above expressions we have symmetrised the matrix elements so that

$$M^{(i)}_{k,q} = M^{(i)}_{-k,q}. \qquad \text{(A3)}$$

This leaves the interaction Hamiltonian invariant, since k and k' are summed over, and the boson operators involving k (or k') in the interaction commute within themselves.

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