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# Two-magnon bound states in the triangular ferromagnet

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**Abstract.** Two-magnon bound states are exact eigenstates of the Heisenberg ferromagnet whose energy falls outside the two-magnon continuum. The well-grounded expectation that at least one bound state exists for any wave vector in 2D Heisenberg ferromagnets seems to be violated when numerical calculations are performed in the triangular lattice. In contrast we show analytically that such a result is a spurious consequence of the numerical computation and we are able to prove that a bound state exists below the two-magnon band for all wave vectors in the triangular ferromagnet.

## 1. Introduction

Two-magnon bound states are exact eigenstates of the Heisenberg ferromagnet. Wortis [1] proved that at least one bound state exists for any wave vector in the 1D Heisenberg ferromagnetic chain and in the 2D square ferromagnet, while in the simple cubic lattice bound states exist below the two-magnon continuum only close to the zone boundary. An intriguing, even though not rigorous, argument of Mattis [2] suggests that bound states in 2D Heisenberg ferromagnets should exist for any wave vector. Recently we have suggested [3] that the existence of a two-magnon bound state at long wavelengths could be a reliable signal of the absence of long range order (LRO). This is true in the 1D and 2D square ferromagnets where exact calculations of two-magnon bound states have been performed and where LRO is absent as required by the Mermin and Wagner theorem [4]. An apparent violation of the thumb rule we have proposed [3] is found in the triangular ferromagnet, where LRO is certainly absent, even though no bound states are found in the neighbourhood of the zone centre [5]. It is worth noticing that the condition for the existence of bound states given in [5] is exact, but the actual solution has been obtained by numerical evaluation of the involved integrals. This calculation is reliable when the bound state energy is sufficiently far from the bottom of the two-magnon band, but we have realized that this procedure becomes meaningless when the bound state is exponentially close to the bottom as occurs in *all* two-dimensional lattices near the zone centre. Note that the numerical investigation of the bound state at small wave vectors should also fail in the 2D square lattice where its occurrence is well established [1, 6]. In the triangular lattice we find that the bound state energy $\hbar\omega_{\rm BS}$ of wave vector $\boldsymbol{K}$ in the neighbourhood of the zone centre is given by

$$\hbar\omega_{\rm BS} = 8JS\left(\tfrac{3}{16}K^2 - \exp(-64\pi S/\sqrt{3}K^2)\right) \qquad (1.1)$$

where the first term on the right is the energy at the bottom of the two-magnon continuum. Equation (1.1) clearly shows why any numerical calculation fails close to the zone centre. The occurrence of the bound state below the bottom of the continuum is beyond any numerical accuracy. So we conclude that only an analytic calculation can detect a bound state in the neighbourhood of the zone centre, as confirmed in the 2D square Heisenberg ferromagnet [1, 6].

## 2. Two-magnon bound states in the triangular lattice

In this section we prove the existence of two-magnon bound states for any wave vector in a triangular Heisenberg ferromagnet. The Hamiltonian we consider reads

$$\mathcal{H} = -J \sum_{i,\delta} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+\delta} \tag{2.1}$$

where $i$ labels the sites of a triangular lattice, $\delta$ joins the site $i$ with its six nearest neighbours (NN), $\boldsymbol{S}_i$ is the spin localized on the site $i$ and $J > 0$ is the ferromagnetic NN exchange coupling. The two-magnon eigenstate $|\boldsymbol{K}\rangle$ for the bosonic equivalent Hamiltonian, obtained from the Heisenberg Hamiltonian (2.1) by the Dyson–Maleev transformation [7], reads

$$|\boldsymbol{K}\rangle = \sum_{\boldsymbol{q}} f_{\boldsymbol{K}}(\boldsymbol{q}) a^\dagger_{\boldsymbol{k}_1} a^\dagger_{\boldsymbol{k}_2} |0\rangle \tag{2.2}$$

where $a^\dagger_{\boldsymbol{k}}$ is the creation operator of a magnon of wave vector $\boldsymbol{k}$,

$$\boldsymbol{k}_1 = \tfrac{1}{2}\boldsymbol{K} + \boldsymbol{q} \qquad \boldsymbol{k}_2 = \tfrac{1}{2}\boldsymbol{K} - \boldsymbol{q} \tag{2.3}$$

and $f_{\boldsymbol{K}}(\boldsymbol{q})$ satisfies the equation

$$\hbar\left(\omega - \omega_{\frac{1}{2}\boldsymbol{K}+\boldsymbol{q}} - \omega_{\frac{1}{2}\boldsymbol{K}-\boldsymbol{q}}\right) f_{\boldsymbol{K}}(\boldsymbol{q}) = 6J\frac{1}{N}\sum_{\boldsymbol{p}}\left(\gamma_{\boldsymbol{q}+\boldsymbol{p}} + \gamma_{\boldsymbol{q}-\boldsymbol{p}} - \gamma_{\frac{1}{2}\boldsymbol{K}+\boldsymbol{q}} - \gamma_{\frac{1}{2}\boldsymbol{K}-\boldsymbol{q}}\right) f_{\boldsymbol{K}}(\boldsymbol{p}) \tag{2.4}$$

where

$$\gamma_{\boldsymbol{q}} = \tfrac{1}{3}\left(\cos q_x + 2\cos\tfrac{1}{2}q_x \cos\tfrac{\sqrt{3}}{2}q_y\right) \tag{2.5}$$

$$\hbar\omega = E - E_0. \tag{2.6}$$

In (2.5) we have assumed the lattice space constant to be unity. In (2.6) $E$ is the eigenvalue of the eigenstate $|\boldsymbol{K}\rangle$ and $E_0$ is the energy of the ferromagnetic ground state $|0\rangle$. The solution of (2.4) is obtained by looking for the zeros of the following determinantal equation

$$\det\left|\delta_{i,j} + \frac{1}{2S}\left(D_{i,j} - D_j \cos\tfrac{1}{2}K_i\right)\right| = 0 \qquad i,j = 1,2,3 \tag{2.7}$$

where

$$D_{i,j} = 8JS\frac{1}{N}\sum_{q}\frac{\cos q_i \cos q_j}{\hbar\omega - \hbar\omega_{\frac{1}{2}K+q} - \hbar\omega_{\frac{1}{2}K-q}} \tag{2.8}$$

$$D_j = 8JS\frac{1}{N}\sum_{q}\frac{\cos q_j}{\hbar\omega - \hbar\omega_{\frac{1}{2}K+q} - \hbar\omega_{\frac{1}{2}K-q}}. \tag{2.9}$$

The magnon dispersion curve reads

$$\hbar\omega_q = 12JS\left[1 - \tfrac{1}{3}\left(\cos q_x + 2\cos\tfrac{1}{2}q_x \cos\tfrac{\sqrt{3}}{2}q_y\right)\right]. \tag{2.10}$$

We look for solutions of (2.7) moving along high symmetry directions like ΓM ($K_x = 0$, $0 < K_y < 2\pi/\sqrt{3}$), ΓX ($0 < K_x < 4\pi/3$, $K_y = 0$) and MX ($0 < K_x < 2\pi/3$, $K_y = 2\pi/\sqrt{3}$). Along these high symmetry directions the possible solutions of (2.7) are given by

$$1 - \frac{1}{2S}I_0 = 0 \tag{2.11a}$$

$$1 - \frac{1}{2S}(I_1 + I_1') + \frac{1}{4S^2}(I_1 I_1' - 2I_2 I_2') = 0. \tag{2.11b}$$

Along the ΓM direction we have

$$I_0 = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \mathrm{d}x\,\mathrm{d}y\,\frac{2\sin^2 x \sin^2 y}{d(\delta, K_y, x, y)} \tag{2.12}$$

with $x = \frac{1}{2}q_x$, $y = \frac{\sqrt{3}}{2}q_y$ and

$$d(\delta, K_y, x, y) = \delta + 2\sin^2 x + 2\cos\tfrac{\sqrt{3}}{4}K_y\,(1 - \cos x \cos y) \tag{2.13}$$

where $\delta$ is the 'binding energy' in units of $8JS$, so that the bound state energy reads

$$\hbar\omega_{\mathrm{BS}} = 16JS\left(1 - \cos\tfrac{\sqrt{3}}{4}K_y\right) - 8JS\delta \tag{2.14}$$

$$I_1 = -\frac{1}{\pi^2}\int_0^\pi\int_0^\pi \mathrm{d}x\,\mathrm{d}y\,\frac{2\sin^2 x \cos 2x}{d(\delta, K_y, x, y)} \tag{2.15}$$

$$I_1' = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \mathrm{d}x\,\mathrm{d}y\,\frac{2\cos x \cos y\left(\cos x \cos y - \cos(\sqrt{3}/4)K_y\right)}{d(\delta, K_y, x, y)} \tag{2.16}$$

$$I_2 = -\frac{1}{\pi^2}\int_0^\pi\int_0^\pi \mathrm{d}x\,\mathrm{d}y\,\frac{2\sin^2 x \cos x \cos y}{d(\delta, K_y, x, y)} \tag{2.17}$$

$$I_2' = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \mathrm{d}x\,\mathrm{d}y\,\frac{\cos 2x\left(\cos x \cos y - \cos(\sqrt{3}/4)K_y\right)}{d(\delta, K_y, x, y)}. \tag{2.18}$$

As one can see, by a direct numerical calculation (2.11*a*) has no solution for any wave vector so that the only bound state along the ΓM direction has to be found as a solution of (2.11*b*). Numerical investigation of (2.11*b*) leads to a bound state for wave vectors in the range $0.55K_y^{ZB} < K_y < K_y^{ZB}$ ($K_y^{ZB} = 2\pi/\sqrt{3}$) in the most favourable case ($S = 1/2$) in agreement with [5], even though the present numerical accuracy is enhanced. Incidentally, at the zone boundary (point M), where the integrals of (2.15)–(2.18) can be evaluated analytically, one finds that the binding energy is

$$\delta = \frac{1}{4S(2S+1)}. \qquad (2.19)$$

For vanishing wave vectors the solution of (2.11*b*) can only be achieved by evaluating analytically the logarithmically divergent contributions of integrals (2.16) and (2.18). In the neighbourhood of the zone centre one has

$$I_1 = \frac{2\sqrt{3}}{\pi} - 1 = 0.102\,657\,8 \qquad (2.20)$$

$$I_1' = \tfrac{1}{2}I_1 - \frac{\sqrt{3}}{32\pi}K_y^2 \ln\delta \qquad (2.21)$$

$$I_2 = -\tfrac{1}{2}I_1 \qquad (2.22)$$

$$I_2' = -\tfrac{1}{2}I_1 - \frac{\sqrt{3}}{64\pi}K_y^2 \ln\delta. \qquad (2.23)$$

Replacing (2.20)–(2.23) in (2.11*b*) one obtains

$$\left(1 - \frac{3}{4S}I_1\right)\left(1 + \frac{1}{2S}\frac{\sqrt{3}}{32\pi}K_y^2 \ln\delta\right) = 0. \qquad (2.24)$$

The first factor of (2.24) never vanishes whereas the second factor leads to a binding energy

$$\delta = \exp\left(-\frac{64\pi S}{\sqrt{3}K_y^2}\right). \qquad (2.25)$$

As one can see, a bound state exists for any wave vector and any $S$ even though the binding energy decreases exponentially as the the wave vector moves towards the zone centre. This exponential decaying of the binding energy for $K_y \to 0$ explains why the numerical approach is hopeless. Note that the numerical solution for $S = 1/2$ is found only in the range $0.55K_y^{ZB} < K_y < K_y^{ZB}$ (at $K_y = 0.55K_y^{ZB}$, $\delta$ is $8.4 \times 10^{-6}$). It is obvious that the value of $\delta$ for vanishing $K_y$ is so small that numerical accuracy is low. For $S > 1/2$ the region is more and more restricted. Let us now comment upon the appealing argument of Mattis [2] supporting the existence of at least one bound state for any wave vector in 2D models. This argument gives the right answer but it is not rigorous since it supports logarithmic divergence of integrals like (2.12) or (2.15)–(2.18) as $\delta \to 0$ caused by the vanishing of the denominators as $K \to 0$. This argument does not take care of the possible vanishing of the numerators which could regularize the integrals. For instance, in the triangular lattice, $I_0$, $I_1$ and $I_2$ are regular, whereas $I_1'$ and $I_2'$ are logarithmically divergent as shown by (2.20)–(2.23). On the other hand this divergence is sufficient to assure the existence of one bound state for all wave vectors along the ΓM direction.

When evaluated for $0 < K_x < 4\pi/3$, $K_y = 0$ (ΓX direction), the integrals appearing in (2.11) become

$$I_0 = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \mathrm{d}x\,\mathrm{d}y\,\frac{2\sin^2 x\sin^2 y}{d(\delta, K_x, x, y)} \tag{2.26}$$

$$I_1 = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \mathrm{d}x\,\mathrm{d}y\,\frac{\cos 2x\,(\cos 2x - \cos\frac{1}{2}K_x)}{d(\delta, K_x, x, y)} \tag{2.27}$$

$$I_1' = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \mathrm{d}x\,\mathrm{d}y\,\frac{2\cos x\cos y\,(\cos x\cos y - \cos\frac{1}{4}K_x)}{d(\delta, K_x, x, y)} \tag{2.28}$$

$$I_2 = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \mathrm{d}x\,\mathrm{d}y\,\frac{\cos 2x\,(\cos x\cos y - \cos\frac{1}{4}K_x)}{d(\delta, K_x, x, y)} \tag{2.29}$$

$$I_2' = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \mathrm{d}x\,\mathrm{d}y\,\frac{\cos x\cos y\,(\cos 2x - \cos\frac{1}{2}K_x)}{d(\delta, K_x, x, y)} \tag{2.30}$$

where

$$d(\delta, K_x, x, y) = \delta + 2\cos\tfrac{1}{2}K_x\sin^2 x + 2\cos\tfrac{1}{4}K_x\,(1-\cos x\cos y) \tag{2.31a}$$

for $0 < K_x < 0.893\,75 K_x^{\mathrm{ZB}}$ ($K_x^{\mathrm{ZB}} = 4\pi/3$) and

$$d(\delta, K_x, x, y) = \delta - 2\cos\tfrac{1}{2}K_x\cos^2 x - \cos\tfrac{1}{4}K_x\left(\frac{\cos\frac{1}{4}K_x}{2\cos\frac{1}{2}K_x} + 2\cos x\cos y\right) \tag{2.31b}$$

for $0.893\,75 K_x^{\mathrm{ZB}} < K_x < K_x^{\mathrm{ZB}}$. The bound state energy reads

$$\hbar\omega_{\mathrm{BS}} = 24JS\left[1 - \tfrac{1}{3}\left(\cos\tfrac{1}{2}K_x + 2\cos\tfrac{1}{4}K_x\right)\right] - 8JS\delta \tag{2.32a}$$

for $0 < K_x < 0.893\,75 K_x^{\mathrm{ZB}}$ and

$$\hbar\omega_{\mathrm{BS}} = 24JS\left[1 + \tfrac{1}{3}\left(\cos\tfrac{1}{2}K_x + \frac{\cos^2\frac{1}{4}K_x}{2\cos\frac{1}{2}K_x}\right)\right] - 8JS\delta \tag{2.32b}$$

for $0.893\,75 K_x^{\mathrm{ZB}} < K_x < K_x^{\mathrm{ZB}}$. The expressions (2.31) for $d(\delta, K_x, x, y)$ and (2.32) for $\hbar\omega_{\mathrm{BS}}$ concerning different ranges of wave vectors, are introduced by the different analytic expression of the lower bound of the two-magnon band and are obtained for the relative wave vectors $\boldsymbol{q} = 0$ or $\boldsymbol{q} = (\arccos[(-\cos K_x/4)/(2\cos K_x/2)], 0)$, respectively. The value $K_x = 0.893\,75 K_x^{\mathrm{ZB}} = 4\arccos\frac{1}{8}(-1+\sqrt{33})$ is the point where these two different determinations cross each other. Equation (2.11$a$) gives a bound state for $S = 1/2$ in the range $0.913\,05 K_x^{\mathrm{ZB}} < K_x < K_x^{\mathrm{ZB}}$ and no bound states for $S \geqslant 1$. On the contrary (2.11$b$) gives a bound state for any $S$ and any wave vector. Once again the numerical solution is found only in the range $0.5K_x^{ZB} < K_x < K_x^{ZB}$ in the most favourable case of $S = 1/2$ (at $K_x = K_x^{ZB}$, $\delta = 3.42\times10^{-5}$ whereas the analytic evaluation of integrals (2.27)–(2.30) close to the zone centre still leads to (2.24) where $K_y$ is replaced by $K_x$. The binding energy is then

$$\delta = \exp\left(-\frac{64\pi S}{\sqrt{3}K_x^2}\right) \tag{2.33}$$

and the bound state energy for $K \to 0$ is given by (1.1).

Along MX ($0 < K_x < 2\pi/3$, $K_y = 2\pi/\sqrt{3}$) the integrals appearing in (2.11) become

$$I_0 = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \mathrm{d}x\,\mathrm{d}y\,\frac{2\cos x\cos y\left(\cos x\cos y - \sin x\sin y + \sin\frac{1}{4}K_x\right)}{d(\delta, K_x, x, y)} \tag{2.34}$$

$$I_1 = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \mathrm{d}x\,\mathrm{d}y\,\frac{\cos 2x\left(\cos 2x - \cos\frac{1}{2}K_x\right)}{d(\delta, K_x, x, y)} \tag{2.35}$$

$$I_1' = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \mathrm{d}x\,\mathrm{d}y\,\frac{2\sin x\sin y\left(\sin x\sin y - \cos x\cos y - \sin\frac{1}{4}K_x\right)}{d(\delta, K_x, x, y)} \tag{2.36}$$

$$I_2 = -\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \mathrm{d}x\,\mathrm{d}y\,\frac{\cos 2x\left(\cos x\cos y - \sin x\sin y + \sin\frac{1}{4}K_x\right)}{d(\delta, K_x, x, y)} \tag{2.37}$$

$$I_2' = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \mathrm{d}x\,\mathrm{d}y\,\frac{(\cos x\cos y - \sin x\sin y)\left(\cos 2x - \cos\frac{1}{2}K_x\right)}{d(\delta, K_x, x, y)} \tag{2.38}$$

where

$$d(\delta, K_x, x, y) = \delta + 2\cos\tfrac{1}{2}K_x\sin^2 x + \sin\tfrac{1}{4}K_x\left(\frac{\sin\frac{1}{4}K_x}{2\cos\frac{1}{2}K_x} - 2\sin x\sin y\right). \tag{2.39}$$

The bound state energy is

$$\hbar\omega_{BS} = 24JS\left[1 - \tfrac{1}{3}\left(\cos\tfrac{1}{2}K_x + \frac{\sin^2\frac{1}{4}K_x}{2\cos\frac{1}{2}K_x}\right)\right] - 8JS\delta. \tag{2.40}$$

Equation (2.11*a*) leads to a bound state for any wave vector between $K_x = 0$ (point M) and $K_x^{ZB} = 2\pi/3$ (point X) for $S = 1/2$ while the range is restricted to $0 < K_x < 0.907\,83K_x^{ZB}$, $0 < K_x < 0.690\,12K_x^{ZB}$, and $0 < K_x < 0.544\,88K_x^{ZB}$, for $S = 1$, $S = 3/2$ and $S = 2$, respectively. Notice that the existence range of this bound state along the MX direction obtained by numerical calculation is reliable, because the integral $I_0$ given by (2.34) is not singular up to the lower bound of the two-magnon band ($\delta = 0$). As one can see, the point A, where this bound state merges with the continuum, jumps discontinuously towards point M as $S$ increases.

This behaviour is analogous to what happens in higher dimensions where the existence region of bound states narrows as $S$ increases.

Equation (2.11*b*) has a solution for any $S$ and any wave vector although the numerical solution is found only for $K_x > 0.2$ as found in [5], even though our numerical accuracy is better. Indeed, integrals (2.35)–(2.38) can be evaluated analytically close to M leading to

$$I_1 = \frac{1}{\sqrt{2\delta}}\frac{3}{32}K_x^2 \qquad (2.41)$$

$$I_1' = \frac{1}{2} - \frac{1}{\sqrt{2\delta}}\frac{1}{32}K_x^2 \qquad (2.42)$$

$$I_2 = \frac{1}{\sqrt{2\delta}}\frac{1}{8}K_x \qquad (2.43)$$

$$I_2' = \tfrac{1}{8}K_x. \qquad (2.44)$$

Replacement of (2.41)–(2.44) in (2.11*b*) gives

$$1 - \frac{1}{4S} - \frac{1}{2S}\left(1 - \frac{1}{8S}\right)\frac{1}{\sqrt{2\delta}}\frac{1}{16}K_x^2 = 0 \qquad (2.45)$$

so that the binding energy is

$$\delta = \frac{1}{32S^2}\left(\frac{8S-1}{4S-1}\right)^2\frac{1}{256}K_x^4. \qquad (2.46)$$

In figure 1 we show the bound states along the high symmetry directions ΓX, XM and ΓM for $S = 1/2$. The inset shows the Brillouin zone of the triangular lattice. For different values of $S$ the scenario is qualitatively unchanged.

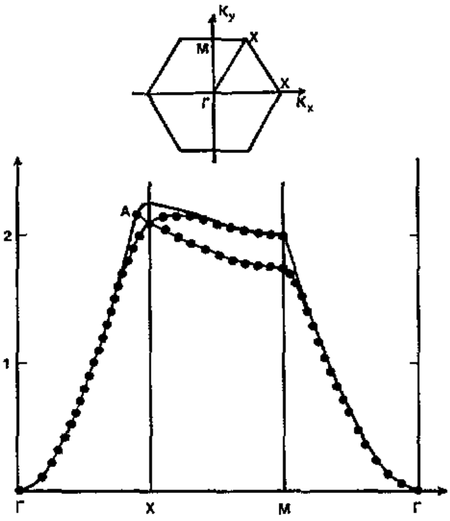


**Figure 1.** Reduced bound state energy $\hbar\omega_{BS}/8JS$ (full circles) as a function of the reduced wave vector along the directions ΓX, XM and ΓM of the triangular ferromagnet with $S = 1/2$. The continuous curve represents the bottom of the two-magnon continuum. The inset shows the Brillouin zone.

## 3. Summary and conclusions

The study of two-magnon bound states in Heisenberg ferromagnets has been widely investigated in the past [8]. Satisfactory results are obtained only for ferromagnets for which the ground state is known and the eigenvalues can be worked out exactly. However, we have found that the actual evaluation of the involved integrals, usually performed numerically [5], is very delicate in 2D systems where at least one bound state exists for all wave vectors even though its binding energy is so small that it can be found only via analytic calculations. We have proved the existence of one bound state over the whole Brillouin zone in the triangular lattice in contrast with previous numerical results [5] and we have also explained the failure of numerical calculation. We conclude that the existence of at least one bound state over the whole Brillouin zone is a genuine feature of all 2D ferromagnetic Heisenberg models in agreement with the Mattis argument [2]. The customary numerical approach, that works well for 3D models and even for large enough wave vectors in 2D models, fails when the bound state is too close to the bottom of the two-magnon continuum. The absence of two-magnon bound states in some regions of the Brillouin zone of the triangular ferromagnet [5] is simply due to insufficient numerical accuracy. We stress that this limitation is strictly related to the nature of the singularity of the integrals and cannot be easily overcome. Analytic testing is necessary. Note that in a 3D model any interlayer coupling $J'$ prevents the divergence of the integrals, so that the numerical evaluation of the bound states becomes reliable. Our conclusion is that two-magnon bound states can be satisfactorily studied in ferromagnetic systems if one proceeds cautiously. On the contrary, in antiferromagnets and helimagnets the situation is much worse because no exact analytic condition for the bound state can be achieved because the exact ground state is unknown. A few approximate results exist for antiferromagnets [9] but nothing at all for helimagnets.

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