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Soliton–magnon bound states in TMMC above and below T_N

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Abstract

The problem of soliton–magnon bound states occurring in the quasi-one-dimensional antiferromagnet TMMC [$(CH_3)_4NMnCL_3$] is studied. Above T_N we found a bound state which is due to out-of-plane spin components when going beyond the sine–Gordon limit. Below T_N we found a bound state which originates from the pairing of π-kinks described by a double-sine–Gordon equation.

The quasi-one-dimensional antiferromagnet TMMC [$(CH_3)_4NMnCl_3$] in the presence of an external magnetic field $\boldsymbol{B}$ can be described by a Hamiltonian H^{3D} of weakly coupled antiferromagnetic chains H_j^{1D} [1,2]:

$$H^{3D} = \sum_j H_j^{1D} - \tfrac{1}{2} J_\perp \sum_{j \neq j'} \sum_l S_{j,l} S_{j',l}, \tag{1}$$

$$H_j^{1D} = \sum_l \Big[J_\parallel S_{j,l} S_{j,l+1} + A\left(S_{j,l}^Z\right)^2 - D\left(S_{j,l}^X\right)^2 - g\mu_B B^X S_{j,l}^X - g\mu_B B^Y S_{j,l}^Y \Big], \tag{2}$$

where the spins $S_{j,l}$ can be treated as classical vectors localized at lattice sites (j_1, j_2, l). The characteristic material parameters fulfill the conditions $J_\parallel \gg A \gg D \gg J_\perp > 0$, moreover we assume $k_B T \ll g\mu_B BS \ll AS^2$ and $J_\perp S^2 \ll (g\mu_B B)^2/4J_\parallel$. Above the Néel temperature T_N interchain interactions are negligible and the system can be described by the 1D Hamiltonian (2). On the other hand it seems reasonable [2] that below T_N the dynamics of the system can be described in terms of an interchain mean field approach [1–3], and as a result, instead of the three-dimensional Hamiltonian (1), we obtain an effective one-dimensional Hamiltonian [1–3] with an interchain mean field $B_{\perp_{MF}}$. In both cases, above and below T_N, the anisotropy term $A(S_{j,l}^Z)^2$ induces the easy XY-plane.

Above T_N the solution of the equations of motion can be found in the form of a π-kink $\Phi_\pi(z)$ [4] which corresponds to a π rotation of spin vectors in the XY-plane. Performing a linear stability analysis for this solution and using a perturbation approach [5] to take into account a coupling between in-plane ($\partial\Phi$) and out-of-plane ($\partial\theta$) fluctuations of spin components, we got a system of two equations:

$$-\partial\Phi_{\zeta\zeta}(\zeta) + \left\{1 - \left[2 + \alpha\omega^2 \cos(2\Delta)\right]\operatorname{sech}^2\zeta + \Delta V(\zeta)\right\}\partial\Phi(\zeta) = \omega^2(1 + \alpha \sin^2\Delta)\partial\Phi(\zeta), \tag{3}$$

$$\partial\theta(\zeta) \approx \frac{b}{4a} \mathrm{i}\Omega \cos\left[\phi_\pi(\zeta) - \gamma\right]\partial\Phi(\zeta), \tag{4}$$

where $a := A/J_\parallel$, $b := g\mu_B B/(J_\parallel S)$, $d := D/J_\parallel$, $\alpha := b^2/(2a) \ll 1$, $\zeta := b_e\, z/2$, $\omega := \Omega/b_e$, Ω is the frequency of the linear perturbations (in units of $J_\parallel S$), b_e is a reduced value of the 'effective' magnetic field given by a solution of the equation $b_e^4 = b^4 - 16db^2\cos(2\gamma) + 64d^2$, γ is the angle between the field $\boldsymbol{B}$ and the X-axis, Δ is the angle between the field $\boldsymbol{B}$ and the direction of the effective field b_e, i.e. $\Delta = \gamma - \beta$, where $\sin(2\beta) = (b/b_e)^2 \sin(2\gamma)$ and the additional potential appearing in Eq. (3) is defined as

$$\Delta V(\zeta) = -\alpha^2\omega \operatorname{sech}\zeta \operatorname{tgh}\zeta \sin(2\Delta).$$

All terms appearing in Eq. (3) that are proportional to the parameter α represent the effect of coupling between in-plane and out-of-plane components.

The solutions of the eigenvalue problem (3) consist of a continuum of delocalized (scattering) states $\partial\Phi_k(\zeta)$ with frequencies starting from $\omega^2(k=0) = 1/(1 + \alpha \sin^2\Delta)$ and a number of bound states with $\omega_b^2 < 1/(1 + \alpha \sin^2\Delta)$. We found that there is only one bound state for $\cos(2\Delta) < 0$ and two bound states for $\cos(2\Delta) > 0$. The single bound state occurring for $\cos(2\Delta) < 0$ and the lower bound state occurring for $\cos(2\Delta) > 0$ correspond to the standard Goldstone mode of a π-kink soliton [6], and their existence is related with the translational invariance of the equations of motions. The frequency of the second bound state (for

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$\cos(2\Delta) > 0$) can be written as

$$\omega_{b,2}^2 \approx \left[1 - \tfrac{1}{9}\alpha^2 \cos^2(2\Delta)\right] / (1 + \alpha \sin^2\Delta), \tag{5}$$

while its shape is given by

$$\partial\Phi_{b,2}(\zeta) \approx \sinh\zeta(\cosh\zeta)^{-1-\epsilon}, \tag{6}$$

where $\epsilon \approx (\alpha/3)\cos(2\Delta)$. It is interesting to note that similar as in the case of out-of-plane effects in the easy-plane ferromagnet [7] the second bound state $\omega_{b,2}^2$ emerges from the continuum threshold $\omega^2(k=0)$. This means, however, that for typical experimental conditions in TMMC, this state occurs very close to the broad uniform mode of spin precession $\omega(k=0)$ and can hardly be detected.

Below the Néel temperature T_N neighbouring spin chains become correlated and the interchain mean field $B_{\perp_{MF}}$ has a nonzero value [1]. A static solution of equations of motion can be written in the form of a 2π-kink $\Phi_{2\pi}(z)$ which is the solution of a double-sine–Gordon equation [1–3]. This 2π-kink has the shape of a pair of coupled π-kinks [8]. Linearizing the equation of motion around this solution we obtained after some approximations

$$-\partial\Phi_{\xi\xi} + \left\{\tanh^2 R\left[2\left(\frac{\sinh^2\xi - \cosh^2 R}{\sinh^2\xi + \cosh^2 R}\right)^2 - 1\right] + \operatorname{sech}^2 R\,\frac{\sinh^2\xi - \cosh^2 R}{\sinh^2\xi + \cosh^2 R} + \Delta V(\xi)\right\}\partial\Phi(\xi) = \hat{\omega}^2\partial\Phi(\xi), \tag{7}$$

$$\partial\Theta(\xi) \approx \frac{b}{4a}\mathrm{i}\Omega\cos[\Phi_{2\pi}(\xi) - \gamma)]\partial\Phi(\xi), \tag{8}$$

where $\xi = (b_\perp + \frac{1}{4}b_e)^{1/2}z$, the reduced frequency $\hat{\omega}$ is $\hat{\omega} = \Omega(b_e^2 + 4b_\perp)^{-1/2}$, the parameter R defined by $\sinh R = b_e/(2\sqrt{b_\perp})$ denotes half the distance between the centers of both π-kinks forming the 2π-kink $\Phi_{2\pi}(\xi)$ and $b_\perp$ is the reduced value of the interchain field i.e. $b_\perp = 6J_\perp/J_\parallel$. The perturbation potential $\Delta V(\xi)$ describing the effect of coupling between the in-plane and out-of-plane spin components is

$$\Delta V(\xi) = \sin^2\Delta + 4\cos(2\Delta)\left(\frac{\cosh R\sinh\xi}{\cosh^2 R + \sinh^2\xi}\right)^2 - 2\sin(2\Delta)\frac{\cosh R\sinh\xi(\cosh^2 R - \sinh^2\xi)}{(\cosh^2 R + \sinh^2\xi)^2}. \tag{9}$$

Similarly as for Eq. (3) the spectrum of Eq. (7) consists of a continuum of scattering states and two bound states. One of these bound states has zero frequency and corresponds to the translational Goldstone mode of the system. The second bound state is connected with an internal oscillation of the 2π-kink, where the center of mass of the 2π-kink does not move but the distance between the centers of both π-kinks oscillates in time. The excitation of these oscillations can influence the thermodynamical properties of the soliton gas [9]. The corresponding frequency $\hat{\omega}_{b,2}$ ranges from zero up to the lower edge of the spin-wave continuum which is given by $\hat{\omega}^2(k=0) = 1/(1 + \alpha\sin^2\Delta)$ in our units. The limit $\hat{\omega}_{b,2} \to 0$ corresponds to the situation where the interchain mean field disappears and the gas of 2π-kinks dissociates into a gas of π-kinks close to the ordering temperature T_N. The approximate expression for the frequency of this bound state, which is valid for intermediate and large distances ($R \geq 1$) between the centers of π-kink pairs, can be written as

$$\hat{\omega}_{b,2}^2 \approx \frac{\dfrac{3}{\sinh^2 R} - \dfrac{1}{\cosh^2 R}\,\dfrac{\sinh(2R) + 2R}{\sinh(2R) - 2R}}{1 + \alpha\left[\cos(2\Delta)g(R) + \sin^2\Delta\right]}, \tag{10}$$

where $g(R)$ is a smoothly varying function [5] taking its maximal value $\frac{2}{3}$ in the limit $R \to \infty$.

In conclusion, we have found analytic expressions for the frequencies of the soliton–magnon bound states in TMMC above and below T_N. The physical reasons for appearing of these states are out-of-plane corrections to equations of motion above T_N and soliton–soliton coupling below T_N.

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