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Coupled Solitons in Alternating Heisenberg Ferromagnetic Chains with a Small Magnon Band Gap *

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The coupled soliton excitations in an alternating Heisenberg ferromagnetic chain with a small magnon band gap are considered. Based on a quasi-discrete multiple scale approach, a set of coupled mode equations is derived which describes the dynamics of strongly coupled acoustic upper cut-off and optical lower cut-off modes. Coupled magnetic band gap soliton solutions are explicitly provided and their frequency properties are discussed.

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In recent years, much effort has been devoted to the experimental and theoretical investigations of nonlinear localized excitations in magnetic systems.[1] Because the earlier research on soliton-like excitations in Heisenberg chains involved a continuum approximation,[2] valid only for long wavelength excitations, many important nonlinear modes with rather short wavelengths were lost.[3] Note that the Heisenberg model describing magnetic phenomena is *inherently* discrete, with lattice spacing being a fundamental physical parameter. An accurate microscopic description for such discrete systems involves a set of difference-differential equations and the intrinsic discreteness may drastically modify the nonlinear dynamics of the systems. The discreteness makes the properties of the system periodic, thus due to the interplay between the discreteness and nonlinearity some new types of intrinsic localized magnon modes, absent in the continuum approximation, may exist.[4] Recently, such nonlinear localized modes have been observed experimentally in $(C_2H_5NH_3)_2CuCl_4$.[5]

In recent years, an increased interest has also been shown in studying the linear and nonlinear excitations in alternating Heisenberg chains (AHCs). Here, an AHC means that the exchange interaction constant (or spin length) in the chain is changed alternatively as $\cdots J_1 - J_2 - J_1 - J_2 \cdots$ (or $\cdots S_1 - S_2 - S_1 - S_2 \cdots$). The AHCs may be realized in many physical systems such as, for example, the layered materials grown by molecular beam epitaxy,[6] dimerized atomic chains through the spin-Peierls effect,[7] and some molecular magnets.[8] Due to the alternation and the discreteness, the magnon frequency spectrum of the system splits into two bands, i.e. the acoustical and the optical bands. In the linear approach, no spin wave can propagate in the gap between the two bands and hence the band gap is also called a stop (or forbidden) band. The situation is, however, changed drastically when the amplitude of a spin excitation is significant. Some new types of nonlinear localized magnon modes, e.g. magnetic gap solitons, can appear in the magnon band gap.[4]

In a recent work the coupling of two magnetic gap solitons was considered in an alternating Heisenberg ferromagnetic chain (AHFC) with a wide band gap.[9] In that case, however, the interaction between two gap solitons is mainly due to the cross-phase modulation and hence the coupling belongs to a weak one. Thus a question arises: what will happen if the band gap width becomes small? It is just this problem that will be addressed here. Note that small band gap AHCs are more realistic for most materials (see Ref. [7]). Since in the case of a small gap the acoustic upper cut-off and the optical lower cut-off modes have almost the same (i.e. degenerate) frequency, the coupling between the two modes is very *strong* so that new types of coupled gap solitons are expected.

The system we study is the one-dimensional AHFC with a Hamiltonian

$$H = -\sum_i J_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - \sum_i D_i (S_i^z)^2 - g\mu_{\rm B} B \sum_i S_i^z, \tag{1}$$

where $\boldsymbol{S}_i = (S_i^x, S_i^y, S_i^z)$ is the spin operator on the site i with spin length independent of i, $J_i = J_1\delta_{i,2j} + J_2\delta_{i,2j+1} (J_2 > J_1 > 0)$ are (alternating) exchange constants where j is an integer. $D_i = D_1\delta_{i,2j} + D_2\delta_{i,2j+1} (D_2 > D_1 > 0)$ is the uniaxial crystal-field anisotropy parameter and B is the external magnetic field applied in the z-direction. (Note that, in the case of an alternating spin length, the Hamiltonian can also be written in the form (1) by a suitable transformation.) The ground-state configuration of the system corresponds to all spins aligned in the z-direction.

We assume that $|S, M\rangle$ is the common eigenstate of the operators $\boldsymbol{S}_i^2$ and S_i^z, where S is the spin

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magnitude and $M\,(=-S,-S+1,\cdots,S-1,S)$ is the eigenvalue of S_i^z. Thus the ground state of the spin at site i is $|0\rangle_i=|S,S\rangle_i$. The $SU(2)$ coherent state $|\zeta_i\rangle$ associated with the spin $\boldsymbol{S}_i$ is given by $|\zeta_i\rangle=(1+|\zeta_i|^2)^{-S}\exp(\zeta_i S_i^-)|0\rangle_i$, where $S_i^{\pm}=S_i^x\pm\mathrm{i}S_i^y$ and ζ_i is a complex spin deviation. The $SU(2)$ coherent state of the system can be constructed by $|\Psi\rangle=\Pi_i|\zeta_i\rangle$. Applying the path-integral theory combined with a stationary phase approximation,[4] the Heisenberg equation of motion for spin $\boldsymbol{S}_i$ is transferred into

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\zeta_i=\sigma_i\zeta_i-S(J_i\zeta_{i+1}+J_{i-1}\zeta_{i-1})+U(\zeta_i,\zeta_{i\pm1}),\quad(2)$$

with $\sigma_i=S(J_1+J_2)+(2S-1)D_i+g\mu_{\mathrm{B}}B$. Here, for simplicity, we have taken $\hbar=1$. U is a nonlinear function of ζ_i and $\zeta_{i\pm1}$ which is not written down explicitly here.

Because of the alternation, the system splits into two sublattices A and B with

$$\begin{aligned}A&=\{\cdots,\boldsymbol{S}_{2i-2},\boldsymbol{S}_{2i},\boldsymbol{S}_{2i+2},\cdots\}\\&=\{\cdots,\boldsymbol{S}_{a,n-1},\boldsymbol{S}_{a,n},\boldsymbol{S}_{a,n+1},\cdots\},\\B&=\{\cdots,\boldsymbol{S}_{2i-1},\boldsymbol{S}_{2i+1},\boldsymbol{S}_{2i+3},\cdots\}\\&=\{\cdots,\boldsymbol{S}_{b,n-1},\boldsymbol{S}_{b,n},\boldsymbol{S}_{b,n+1},\cdots\},\end{aligned}$$

where n is the index of nth unit cell with lattice constant $a=2a_0$, and a_0 is the spacing between two nearest-neighbour spins. Hence Eq. (2) reads

$$\begin{aligned}\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\phi_n=&\,\sigma_1\phi_n-S(J_1\psi_n+J_2\psi_{n-1})\\&+U_1(J_1,J_2,D_1,\phi_n,\psi_n,\psi_{n-1}),\qquad(3)\\\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi_n=&\,\sigma_2\psi_n-S(J_1\phi_n+J_2\phi_{n+1})\\&+U_2(J_1,J_2,D_2,\phi_n,\psi_n,\phi_{n+1}),\qquad(4)\end{aligned}$$

where $\phi_n=\zeta_{2i}$, $\psi_n=\zeta_{2i+1}$ and U_1 and U_2 are the two nonlinear functions.

Assuming that

$$\begin{pmatrix}\phi_n\\\psi_n\end{pmatrix}=\epsilon\begin{pmatrix}\phi_0\\\psi_0\end{pmatrix}\exp[\mathrm{i}(qna-\omega t)]$$

where ϕ_0 and ψ_0 are constants and ϵ is a small parameter, one obtains the linear dispersion relation of the system:

$$\begin{aligned}\omega_{\pm}(q)=&\,\frac{1}{2}\{\sigma_1+\sigma_2\pm[(\sigma_2-\sigma_1)^2\\&+4S^2[J_1^2+J_2^2+2J_1J_2\cos(qa)]]^{1/2}\}.\end{aligned}\quad(5)$$

We see that the magnon frequency spectrum of the AHFC displays two branches. One is the acoustic band $\omega_-(q)$ and the other is the optical band $\omega_+(q)$. At $q=\pi/a$ a *frequency band gap* exists between the upper cut-off of the acoustic band ω_1, and the lower cut-off of the optical band ω_2, with $\omega_1\equiv\omega_-(\pi/a)=\{\sigma_1+\sigma_2-[(\sigma_2-\sigma_1)^2+4S^2(J_2-J_1)^2]^{1/2}\}/2$ and $\omega_2\equiv\omega_+(\pi/a)=\{\sigma_1+\sigma_2+[(\sigma_2-\sigma_1)^2+4S^2(J_2-J_1)^2]^{1/2}\}/2$. The band gap width is

$$\omega_2-\omega_1=[(2S-1)^2(D_2-D_1)^2+4S^2(J_2-J_1)^2]^{1/2}.\quad(6)$$

In linear theory, the propagation of a spin wave in the band gap (i.e. stop band) is forbidden. The situation is, however, changed drastically when the nonlinear effect is significant. Some nonlinear localized modes may appear in the band gap.[4] Here our main interest is in strong nonlinear coupling between the acoustic upper cut-off and the optical lower cut-off modes. To this end we first make the asymptotic expansion[10] $u_n(t)=\epsilon u^{(1)}(\xi_n,\tau;\theta_n)+\epsilon^2u^{(2)}(\xi_n,\tau;\theta_n)+\cdots=\sum_{\nu=1}^{\infty}\epsilon^\nu u_{n,n}^{(\nu)}$, where $u_n(t)$ represents $\phi_n(t)$ or $\psi_n(t)$ and $u_{n,n}^{(\nu)}$ represents $u^{(\nu)}(\xi_n,\tau;\theta_n)$ with $\xi_n=\epsilon^2na$ and $\tau=\epsilon^2t$ (slow variables) and $\theta_n=qna-\omega t$ (fast variable). For a small gap we assume $J_1=J-\epsilon^2\alpha_1$, $J_2=J+\epsilon^2\alpha_1$, $D_1=D-\epsilon^2\alpha_2$ and $D_2=D+\epsilon^2\alpha_2$ with $\alpha_j\,(j=1,2)$ of the order of unity. The gap width (Eq. (6)) is now given by

$$\omega_2-\omega_1=2\epsilon[4S^2\alpha_1^2+(2S-1)^2\alpha_2^2]^{1/2}.\qquad(7)$$

Thus we have the small gap with its width characterized by the small parameter ϵ. With these considerations, Eqs. (2) and (3) are transformed into a hierarchy of equations for $\phi_{n,n}^{(\nu)}$ and $\psi_{n,n}^{(\nu)}$ by equating the coefficients of the same powers of ϵ.

In the leading order ($\nu=1$), the solution representing the excitation of the acoustic upper cut-off and the optical lower cut-off modes reads

$$\begin{aligned}\phi_{n,n}^{(1)}&=A_-(\xi_n,\tau)(-1)^n\exp(-\mathrm{i}\omega_0t),\\\psi_{n,n}^{(1)}&=A_+(\xi_n,\tau)(-1)^n\exp(-\mathrm{i}\omega_0t),\end{aligned}\qquad(8)$$

where $\omega_0=2JS+(2S-1)D+g\mu_{\mathrm{B}}B$. Keeping the perturbation expansion to the third order ($\nu=3$) the solvability conditions yield the equations controlling the envelopes $A_{\pm}$:

$$\begin{aligned}&\mathrm{i}\frac{\partial A_1}{\partial t}+JSa\frac{\partial A_2}{\partial x_n}+2D(2S-1)|A_1|^2A_1\\&\quad+4JS|A_2|^2A_1+(2S-1)\tilde{\alpha_2}A_1-2S\tilde{\alpha_1}A_2=0,\end{aligned}\qquad(9)$$

$$\begin{aligned}&\mathrm{i}\frac{\partial A_2}{\partial t}-JSa\frac{\partial A_1}{\partial x_n}+4JS|A_1|^2A_2+2D(2S-1)\\&\quad\cdot|A_2|^2A_2-2S\tilde{\alpha_1}A_1-(2S-1)\tilde{\alpha_2}A_2=0,\end{aligned}\qquad(10)$$

when returning to the original variables, where $A_1=\epsilon A_-$, $A_2=\epsilon A_+$ and $\tilde{\alpha_j}=\epsilon^2\alpha_j\,(j=1,2)$. Note that the self-phase modulation terms $(|A_j|^2A_j, j=1,2)$ result from the uniaxial anisotropy while the cross-phase modulation terms $(|A_j|^2A_{3-j})$ come from the exchange interaction.

Next we consider possible coupled soliton solutions of the coupled-mode Eqs. (9) and (10). We take

$A_j(x_n,t) = f_j(x_n)\exp(-\mathrm{i}\Omega t)(j=1,2)$ where f_j is the real function and Ω is a real constant. Then Eqs. (9) and (10) become

$$\frac{\mathrm{d}f_1}{\mathrm{d}z} = -\eta f_1 - \eta_1 f_2 + \eta_3 f_1^2 f_2 + \eta_4 f_2^3, \quad (11)$$

$$\frac{\mathrm{d}f_2}{\mathrm{d}z} = \eta f_2 - \eta_2 f_1 - \eta_3 f_2^2 f_1 - \eta_4 f_1^3, \quad (12)$$

with $z = x_n/(JSa)$, $\eta = 2S\tilde{\alpha_1}$, $\eta_1 = -\Omega + (2S-1)\tilde{\alpha_2}$, $\eta_2 = -\Omega - (2S-1)\tilde{\alpha_2}$, $\eta_3 = 4JS$ and $\eta_4 = 2(2S-1)D$. Equations (11) and (12) form a dynamical system with the Hamiltonian $\mathcal{H} = -(1/2)(\eta_2 f_1^2 + \eta_1 f_2^2 + 2\eta f_1 f_2) + (1/2)\eta_3 f_1^2 f_2^2 + (1/4)\eta_4(f_1^4 + f_2^4)$. By introducing the function $h(z) = f_1(z)/f_2(z)$, Eqs. (11) and (12) can be solved exactly by integrating the equation $\mathrm{d}h/\mathrm{d}z = \pm[(\eta_1 + 2\eta h + \eta_2 h^2)^{1/2}$, where E is the value of the "energy" corresponding to the particular orbit in the phase space (f_1, f_2) associated with $\mathcal{H}$. The solutions for f_1 and f_2 can be found through the relation $f_1 = hf_2$, $f_2^2 = \{\eta_1 + 2\eta h + \eta_2 h^2 \pm [(\eta_1 + 2\eta h + \eta_2 h^2)^2 + 4E(\eta_4 + 2\eta_3 h^2 + \eta_4 h^4)]^{1/2}/(\eta_4 + 2\eta_3 h^2 + \eta_4 h^4)$. We find that Ω *is an important detuning (bifurcation) parameter controlling the type of coupled soliton solutions.* Two types of solution corresponding to $E = 0$ are found for different values of Ω.

(1) In the region $-\Omega_1 < \Omega < -\Omega_0$, where $\Omega_0 = (2S-1)\tilde{\alpha_2}$ and $\Omega_1 = \{[2S-1)\tilde{\alpha_2}]^2 + 4S^2\tilde{\alpha_1}^2\}^{1/2}$, one has $\eta_2 > 0$ and $\eta^2 - \eta_1\eta_2 > 0$. We obtain $h = \delta_1 r_1 \coth y - \eta/\eta_2$ and hence

$$\begin{aligned} f_1 = {} & \delta_1\delta_2\sqrt{2}r_1 \mathrm{csch} y(\delta_1 r_1 \coth y - \eta/\eta_2) \\ & \cdot\{[\eta_4 + 2\eta_3(\delta_1 r_1 \coth y - \eta/\eta_2)^2 \\ & + \eta_4(\delta_1 r_1 \coth y - \eta/\eta_2)^4]^{1/2}\}^{-1}, \end{aligned} \quad (13)$$

$$\begin{aligned} f_2 = {} & \delta_1\delta_2\sqrt{2}r_1 \mathrm{csch} y\{[\eta_4 + 2\eta_3(\delta_1 r_1 \coth y - \eta/\eta_2)^2 \\ & + \eta_4(\delta_1 r_1 \coth y - \eta/\eta_2)^4]^{1/2}\}^{-1}, \end{aligned} \quad (14)$$

where $y = r(z - z_0)$, $r_1 = r/\sqrt{\eta_2}$ and $\delta_j \pm 1 (j = 1,2)$ with $r = (\eta^2 - \eta_1\eta_2)^{1/2}$ and z_0 an arbitrary constant. We see that both envelopes are bright solitons. However, they are different kinds of bright solitons since the soliton f_1 (the envelope of the acoustic upper cut-off mode) is symmetric with only one maximum but the soliton f_2 (the envelope of the optical lower cut-off mode) is asymmetric and there are two extrema.

(2) In the region $-\Omega_0 < \Omega < \Omega_1$, we have $\eta^2 - \eta_1\eta_2 > 0$ but $\eta_2 < 0$. In this case we find $h = \delta_1 r_2 \tanh y - \eta/\eta_2$ and hence

$$\begin{aligned} f_1 = {} & \delta_2\sqrt{2}r_2 \mathrm{sech} y(\delta_1 r_2 \tanh y - \eta/\eta_2) \\ & \cdot\{[\eta_4 + 2\eta_3(\delta_1 r_2 \tanh y - \eta/\eta_2)^2 \\ & + \eta_4(\delta_1 r_2 \tanh y - \eta/\eta_2)^4]^{1/2}\}^{-1}, \end{aligned} \quad (15)$$

$$\begin{aligned} f_2 = {} & \delta_2\sqrt{2}r_2 \mathrm{sech} y\{[\eta_4 + 2\eta_3(\delta_1 r_2 \tanh y - \eta/\eta_2)^2 \\ & + \eta_4(\delta_1 r_2 \tanh y - \eta/\eta_2)^4]^{1/2}\}^{-1}, \end{aligned} \quad (16)$$

with $r_2 = r/\sqrt{-\eta_2}$. Again, both f_1 and f_2 are bright solitons but in this circumstance f_1 is asymmetric with two extrema while f_2 is symmetric with only one maximum.

Finally, we discuss the frequency property of the coupled solitons obtained above. From Eq. (8), in the leading-order approximation we have $\phi_n = f_1\exp[-\mathrm{i}(\omega_0 + \Omega)t]$ and $\psi_n = f_2\exp[-\mathrm{i}(\omega_0 + \Omega)t]$. Thus both solitons vibrate with the frequency $\omega = \omega_0 + \Omega$. The existence region of the coupled solitons Eqs. (13) and (14), $-\Omega_1 < \Omega < \Omega_0$, means that $\omega_0 - \Omega_1 (= \omega_1) < \omega < \omega_c (\equiv \omega_0 - \Omega_0)$. Thus the vibrating frequency of these coupled solitons is within the *lower part* of the magnon band gap. On the other hand, the existence region of the coupled solitons Eqs. (15) and (16), $-\Omega_0 < \Omega < \Omega_1$, yields $\omega_c < \omega < \omega_2 (= \omega_0 + \Omega_1)$. Hence the vibrating frequency of the coupled solitons Eqs. (15) and (16) is within the *upper part* of the band gap.

In conclusion, based on a quasi-discrete multiple scale approach[10] we have investigated the *strong coupling* of the acoustic upper cut-off and the optical lower cut-off modes in an AHFC. New types of coupled solitons with their vibrating frequency within the magnon band gap have been presented explicitly. We found that in the band gap, there exists a "critical frequency" ω_c. In the lower part of the gap (i.e. $\omega_1 < \omega < \omega_c$) the coupled solitons provided by Eqs. (13) and (14) are possible; while in the upper part of the gap (i.e. $\omega_c < \omega < \omega_2$) the other type of coupled solitons, given by Eqs. (15) and (16), can appear. Note that band gap solitons have been observed experimentally in one-dimensional photonic crystals[11] and in the pendulum lattices.[12] Our results presented above may be useful for further understanding of the excitation spectrum in magnetic systems and as a guide for new experimental findings.

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