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# Coupled Band Gap Solitons in One-Dimensional Alternating Heisenberg Ferromagnetic Chains*

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**Abstract** *The dynamics of coupled band gap solitons in one-dimensional Heisenberg ferromagnetic chains with bond alternation is considered analytically. Using the method of multiple scales the nonlinear coupled-mode equations (i.e. Manakov equations) for the upper cutoff mode of acoustic band and the lower cutoff mode of optical band are derived under the quasi-discreteness approximation. Due to the cross-phase modulation the type of soliton excitations may be changed and the vibrating frequencies of these soliton excitations may locate within or outside the gap of magnon frequency bands.*

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**Key words:** gap solitons, Heisenberg ferromagnetic chains

## 1 Introduction

Recent years have shown increased interest in the study of nonlinear localized excitations in condensed matter systems. Ferromagnetic and antiferromagnetic chain compounds, e.g. $CsNiF_3$ and TMMC $[(CCD_3)_4NM_nCl_3]$, have been shown to be good systems exhibiting soliton-type nonlinear excitations.[1−4] However, since in theory almost all approaches involved the continuum approximations, some nonlinear modes with rather short wavelength have been lost.[5] Note that the Heisenberg model describing magnetic phenomena is ***inherently*** discrete, with the lattice spacing a fundamental physical parameter. For such discrete systems an accurate microscopic description 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, so that due to the interplay between the discreteness and the nonlinearity, certain types of nonlinear excitations which have no direct analog in continuum models, may exist. In fact, some nonlinear localized magnon modes, say intrinsic localized magnon modes, have attracted much recent theoretical attention[6−11] and some of them have been observed experimentally.[12] Lai and Sievers have given a comprehensive review on this subject.[13]

Note that some magnetic systems, e.g. layered materials grown by molecular-beam epitaxy, display strong alternating exchange interaction (i.e. bond alternation).[14,15] Due to the bond alternation and the discreteness of the system, magnon frequency spectrum splits into two bands, i.e. an acoustic and an optical bands. There is band gap between two bands and an upper cutoff frequency for all the bands. In linear theory, spin waves cannot propagate in the band gap. But the situation is changed drastically when the nonlinearity of the system plays a significant role. Some new types of nonlinear localized modes, e.g. spin gap solitons, can appear with their vibrating frequencies in the gap of the magnon bands. References [16] and [17] presented a detailed study on these spin gap solitons.

In view of aforementioned works, we found that up to now almost all studies on magnetic solitons have focused on single-mode excitations. In this paper, we consider the nonlinear ***coupling*** of two magnon modes relevant to the boundary of Brillouin zone. Using the method of multiple scales we derive coupled nonlinear envelope equations (i.e. Manakov equations) based on a quasi-discreteness approach.[18−20] Coupled soliton-soliton and soliton-kink solutions are given explicitly and these new types of nonlinear excitations display interesting properties. The paper is organized as follows. In Sec. 2, based on a quasi-discreteness approach developed in Refs [18]–[20], we present the model and make an asymptotic expansion. A set of coupled-mode equations are derived. Section 3 provides coupled soliton solutions and discusses their properties, in particular for their vibrating frequencies. Finally, section 4 contains a summary of our results.

## 2 Model and Asymptotic Expansion

### 2.1 *The Model*

The system we considered is the one-dimensional al-

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ternating Heisenberg ferromagnet with the Hamiltonian

$$H = -\sum_i J_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - \sum_i D_i (S_i^z)^2 - g\mu_B f \sum_i S_i^z \,, \quad (1)$$

where $\boldsymbol{S}_i = (S_i^x, S_i^y, S_i^z)$ is the spin on the site $i$ and $J_j = J_1\delta_{j,2i} + J_2\delta_{j,2i+1}$ ($J_2 > J_1 > 0$) is the strength of alternating bonds. $D_j = D_1\delta_{j,2i} + D_2\delta_{j,2i+1}$ ($D_2 > D_1 > 0$) is the uniaxial crystal-field anisotropy parameter and $f$ is the intensity of external magnetic field along $z$-direction. The ground-state configuration of the system corresponds to all spins aligned in the $z$-axis direction.

Assume that $|S, M\rangle$ is the common eigenstate of the angular momenta $\boldsymbol{S}_i^2$ and $S_i^z$, where $S$ is the spin magnitude and $M$ (taking values $-S, -S+1, \ldots, S-1, S$) 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[16,21]

$$|\zeta_i\rangle = (1 + |\zeta_i|^2)^{-S} \exp(\zeta_i S_i^-)|0\rangle_i \,, \quad (2)$$

where $S_i^\pm = S_i^x \pm \mathrm{i} S_i^y$ and $\zeta_i$ is a complex spin deviation defined as a magnon field variable. The SU(2) coherent state of the system constituting the ferromagnetic chain with bond alternation can be constructed by

$$|\Psi\rangle = \Pi_i |\zeta_i\rangle \,. \quad (3)$$

Applying the path-integral theory combined with a stationary phase approximation[7] the Heisenberg equation of motion for spin $\boldsymbol{S}_i$ is transferred into the following one

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\zeta_i = \sigma_i\zeta_i - S(J_i\zeta_{i+1} + J_{i-1}\zeta_{i-1}) + U(\zeta_i, \zeta_{i\pm1}) \quad (4)$$

with

$$\sigma_i = S(J_1 + J_2) + (2S-1)D_i + g\mu_B f \,, \quad (5)$$

$$\begin{aligned} U = {} & J_i S(|\zeta_{i+1}|^2\zeta_{i+1} + \zeta_{i+1}^*\zeta_i^2 - 2|\zeta_{i+1}|^2\zeta_i)/(1 + |\zeta_{i+1}|^2) \\ & + J_{i-1}S(|\zeta_{i-1}|^2\zeta_{i-1} + \zeta_{i-1}^*\zeta_i^2 \\ & - 2|\zeta_{i-1}|^2\zeta_i)/(1 + |\zeta_{i-1}|^2) \\ & - 2D_i(2S-1)|\zeta_i|^2\zeta_i/(1 + |\zeta_i|^2) \,, \end{aligned} \quad (6)$$

here for simplicity we have taken $\hbar = 1$.

The alternating bond splits the system into two sublattices $A$ and $B$ with

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

(even spins) and

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

(odd spins), where $n$ is the index of $n$th unit cell with lattice constant $a = 2a_0$, $a_0$ is the spacing between two nearest-neighbor spins. Then the coherent state amplitude equation (4) becomes

$$\begin{aligned} \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\phi_n = {} & \sigma_1\phi_n - S(J_1\psi_n + J_2\psi_{n-1}) + J_1 S(\psi_n|\psi_n|^2 + \phi_n^2\psi_n^* - 2\phi_n|\psi_n|^2)/(1 + |\psi_n|^2) + J_2 S(\psi_{n-1}|\psi_{n-1}|^2 \\ & + \phi_n^2\psi_{n-1}^* - 2\phi_n|\psi_{n-1}|^2)/(1 + |\psi_{n-1}|^2) - 2D_1(2S-1)\phi_n|\phi_n|^2/(1 + |\phi_n|^2) \,, \end{aligned} \quad (7)$$

$$\begin{aligned} \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi_n = {} & \sigma_2\psi_n - S(J_1\phi_n + J_2\phi_{n+1}) + J_1 S(\phi_n|\phi_n|^2 + \psi_n^2\phi_n^* - 2\psi_n|\phi_n|^2)/(1 + |\phi_n|^2) + J_2 S(\phi_{n+1}|\phi_{n+1}|^2 \\ & + \psi_n^2\phi_{n+1}^* - 2\psi_n|\phi_{n+1}|^2)/(1 + |\phi_{n+1}|^2) - 2D_2(2S-1)\psi_n|\psi_n|^2/(1 + |\psi_n|^2) \,, \end{aligned} \quad (8)$$

where $\phi_n = \zeta_{2i}$, $\psi_n = \zeta_{2i+1}$.

### 2.2 *Asymptotic Expansion*

The conventionally used analytical approach for coherent state amplitude equations involved the continuum approximation. This procedure is valid only for long wavelength excitations. Genuine modes of the discreteness of the system are lost in such a treatment. Here we take the quasi-discreteness approach developed in Refs [18]–[20] to investigate the coupling between two cutoff modes of spin wave relevant to the boundary of the Brillouin zone. The carrier waves of these cutoff modes vary fast thus have fairly short wavelength. To this aim we make the expansion

$$\begin{aligned} u_n(t) &= \epsilon u^{(1)}(\xi_n, \tau; \theta_n) + \epsilon^2 u^{(2)}(\xi_n, \tau; \theta_n) + \cdots \\ &= \sum_{\nu=1}^{\infty} u_{n,n}^{(\nu)} \,, \end{aligned} \quad (9)$$

where $u_n(t)$ represents $\phi_n(t)$ or $\psi_n(t)$. The quantity $\epsilon$ is a smallness but finite parameter denoting the magnitude of the amplitude of the excitation and $u_{n,n}^{(\nu)} \equiv u^{(\nu)}(\xi_n, \tau; \theta_n)$ with $\xi_n = \epsilon(na - \lambda t)$ and $\tau = \epsilon^2 t$ (slow variables). $\lambda$ is a parameter to be determined by a solvability condition. The fast variable, $\xi_n = qna - \omega t$, representing the phase of the carrier wave, is taken to be completely discrete. Substituting Eq. (9) into Eqs (7) and (8) and comparing the coefficients of the same powers of $\epsilon$, one obtains

$$\Big(\mathrm{i}\frac{\partial}{\partial t} - \sigma_1\Big)\phi_{n,n}^{(j)} + S(J_1\psi_{n,n}^{(j)} + J_2\psi_{n,n-1}^{(j)}) = M_{n,n}^{(j)} \,, \quad (10)$$

$$M_{n,n}^{(1)} = 0 \,, \quad (11)$$

$$M_{n,n}^{(2)} = \mathrm{i}\lambda \frac{\partial}{\partial \xi_n}\phi_{n,n}^{(1)} + J_2 Sa \frac{\partial}{\partial \xi_n}\psi_{n,n-1}^{(1)}\,, \tag{12}$$

$$M_{n,n}^{(3)} = \cdots\,, \tag{13}$$

and

$$\Big(\mathrm{i}\frac{\partial}{\partial t} - \sigma_2\Big)\psi_{n,n}^{(j)} + S(J_1\phi_{n,n}^{(j)} + J_2\phi_{n,n+1}^{(j)}) = N_{n,n}^{(j)}\,, \tag{14}$$

$$N_{n,n}^{(1)} = 0\,, \tag{15}$$

$$N_{n,n}^{(2)} = \mathrm{i}\lambda \frac{\partial}{\partial \xi_n}\psi_{n,n}^{(1)} + J_2 Sa \frac{\partial}{\partial \xi_n}\phi_{n,n+1}^{(1)}\,, \tag{16}$$

$$N_{n,n}^{(3)} = \cdots \tag{17}$$

with $j = 1, 2, 3, \ldots$. The expressions of $M_{n,n}^{(j)}$ and $N_{n,n}^{(j)}$ ($j = 3, 4, \ldots$) are not explicitly written down here.

### 2.3 *Coupled-Mode Equations*

Now we derive coupled-mode equations starting from Eqs (10) $\sim$ (17). For $j = 1$ it is easy to get

$$\phi_{n,n}^{(1)} = A_-(\xi_n,\tau)\exp(\mathrm{i}\theta_n^-) - \frac{S[J_1 + J_2\exp(-\mathrm{i}qa)]}{\omega_+(q) - \sigma_1}A_+(\xi_n,\tau)\exp(\mathrm{i}\theta_n^+)\,, \tag{18}$$

$$\psi_{n,n}^{(1)} = -\frac{S[J_1 + J_2\exp(\mathrm{i}qa)]}{\omega_-(q) - \sigma_2}A_-(\xi_n,\tau)\exp(\mathrm{i}\theta_n^-) + A_+(\xi_n,\tau)\exp(\mathrm{i}\theta_n^+)\,, \tag{19}$$

where $A_-$ and $A_+$ are two envelope (or amplitude) functions yet to be determined. $\theta_n^{\pm} = qna - \omega_{\pm}(q)t$ are the phases of the carrier waves for the acoustic (minus sign) and the optical (plus sign) modes. $\omega_{\pm}$ are given by

$$\omega_{\pm}(q) = \frac{1}{2}\{\sigma_1 + \sigma_2 \pm [(\sigma_2 - \sigma_1)^2 + 4S^2[J_1^2 + J_2^2 + 2J_1J_2\cos(qa)]\,]^{1/2}\}\,. \tag{20}$$

Thus we see that the magnon frequency spectrum of the Heisenberg ferromagnetic chain with bond alternation displays two branches. One is the lower branch $\omega_-(q)$ (the acoustic branch) and the other is the upper branch $\omega_+(q)$ (the optical branch). At $q = 0$ the eigenfrequency spectrum has a lower cutoff

$$\omega_-(0) = (1/2)\{\sigma_1 + \sigma_2 - [(\sigma_2 - \sigma_1)^2 + 4S^2(J_1 + J_2)^2]^{1/2}\}$$

for the acoustic mode and an upper cutoff

$$\omega_+(0) = (1/2)\{\sigma_1 + \sigma_2 + [(\sigma_2 - \sigma_1)^2 + 4S^2(J_1 + J_2)^2]^{1/2}\}$$

for the optical mode. At $q = \pi/a$ there exists a ***frequency gap*** between the upper cutoff of the acoustic band, $\omega_1$, and the lower cutoff of the optical band, $\omega_2$, with

$$\omega_1 \equiv \omega_-(\pi/a) = \frac{1}{2}\{\sigma_1 + \sigma_2 - [(\sigma_2 - \sigma_1)^2 + 4S^2(J_2 - J_1)^2]^{1/2}\}\,, \tag{21}$$

$$\omega_2 \equiv \omega_+(\pi/a) = \frac{1}{2}\{\sigma_1 + \sigma_2 + [(\sigma_2 - \sigma_1)^2 + 4S^2(J_2 - J_1)^2]^{1/2}\}\,. \tag{22}$$

The band gap width is

$$\omega_2 - \omega_1 = [(\sigma_2 - \sigma_1)^2 + 4S^2(J_2 - J_1)^2]^{1/2} = [(2S - 1)^2(D_2 - D_1)^2 + 4S^2(J_2 - J_1)^2]^{1/2}. \tag{23}$$

In linear theory, the frequency gap is a "forbidden band (or stop band)" for the spin waves. However, if the amplitude of the spin waves is significant, nonlinearity of the system cannot be neglected. Some nonlinear localized spin wave modes may appear in the band gap. Reference [16] has studied the nonlinear single-mode excitations with the vibrating frequencies within or outside the gap. Here we are interested in the nonlinear coupling between the acoustic upper cutoff mode and the optical lower cutoff mode. To this end we take $q$ (the wave number of the carrier wave) to be $\pi/a$ and hence equations (18) and (19) become

$$\phi_{n,n}^{(1)} = A_-(\xi_n,\tau)(-1)^n\exp(-\mathrm{i}\omega_1 t) + \frac{S(J_2 - J_1)}{\omega_2 - \sigma_1}A_+(\xi_n,\tau)(-1)^n\exp(-\mathrm{i}\omega_2 t)\,, \tag{24}$$

$$\psi_{n,n}^{(1)} = \frac{S(J_2 - J_1)}{\omega_1 - \sigma_2}A_-(\xi_n,\tau)(-1)^n\exp(-\mathrm{i}\omega_1 t) + A_+(\xi_n,\tau)(-1)^n\exp(-\mathrm{i}\omega_2 t)\,. \tag{25}$$

In the next order ($j = 2$), a solvability condition demands $\lambda = 0$ and hence $\xi_n = \epsilon na \equiv x_n$. This is a quite natural result because the cutoff modes have vanishing group velocity. The solution in this order is given by

$$\phi_{n,n}^{(2)} = -\frac{J_2 Sa}{\omega_2 - \sigma_1}\frac{\partial A_+}{\partial \xi_n}(-1)^n\exp(-\mathrm{i}\omega_2 t)\,, \tag{26}$$

$$\psi_{n,n}^{(1)} = \frac{J_2 Sa}{\omega_1 - \sigma_2}\frac{\partial A_-}{\partial \xi_n}(-1)^n\exp(-\mathrm{i}\omega_1 t)\,. \tag{27}$$

With the results obtained in Eqs (24) $\sim$ (27) one can calculate $M_{n,n}^{(3)}$ and $N_{n,n}^{(3)}$. The solvability conditions of Eqs (10) and (14) with $j = 3$ yield the closed equations for $A_-$ and $A_+$,

$$\mathrm{i}\frac{\partial A_1}{\partial t} - \beta\frac{\partial^2 A_1}{\partial x_n^2} + P_1|A_1|^2A_1 + Q_1|A_2|^2A_1 = 0\,, \tag{28}$$

$$\mathrm{i}\frac{\partial A_2}{\partial t} + \beta\frac{\partial^2 A_2}{\partial x_n^2} + P_2|A_2|^2A_2 + Q_2|A_1|^2A_2 = 0\,, \tag{29}$$

when returning to original variables, where we have taken $A_1 = \epsilon A_-$ and $A_2 = \epsilon A_+$. The coefficients appearing in Eqs (28) and (29) are given by

$$\beta = \frac{J_1J_2S^2a^2}{[(2S - 1)^2(D_2 - D_1)^2 + 4S^2(J_2 - J_1)^2]^{1/2}}\,, \tag{30}$$

$$P_1 = \frac{-2(\omega_1 - \sigma_1)}{\sigma_1 + \sigma_2 - 2\omega_1}\Big\{2\omega_1 - \sigma_1 - \sigma_2 + 2S(J_1 + J_2) + (2S - 1)\Big[\frac{D_1(\omega_1 - \sigma_2)}{\omega_1 - \sigma_1} + \frac{D_2(\omega_1 - \sigma_1)}{\omega_1 - \sigma_2}\Big]\Big\}\,, \tag{31}$$

$$P_2 = \frac{-2(\omega_2 - \sigma_2)}{\sigma_1 + \sigma_2 - 2\omega_2}\Big\{2\omega_2 - \sigma_1 - \sigma_2 + 2S(J_1 + J_2)$$

$$+ (2S-1)\Big[\frac{D_1(\omega_2-\sigma_2)}{\omega_2-\sigma_1}+\frac{D_2(\omega_2-\sigma_1)}{\omega_2-\sigma_2}\Big]\Big\}\,, \tag{32}$$

$$Q_1 = \frac{2(\omega_2-\sigma_2)}{\sigma_1+\sigma_2-2\omega_1}\Big\{(2S-1)(D_1+D_2)+S(J_1+J_2) \times\Big[\frac{\omega_1-\sigma_2}{\omega_1-\sigma_1}+\frac{S(J_2-J_1)}{\omega_1-\sigma_2}-2\Big]\Big\}\,, \tag{33}$$

$$Q_1 = \frac{2(\omega_1-\sigma_1)}{\sigma_1+\sigma_2-2\omega_2}\Big\{(2S-1)(D_1+D_2)+S(J_1+J_2) \times\Big[\frac{\omega_2-\sigma_1}{\omega_2-\sigma_2}+\frac{S(J_2-J_1)}{\omega_2-\sigma_1}-2\Big]\Big\}\,. \tag{34}$$

Equations (28) and (29) are ***coupled-mode equations*** we sought. They are called the Manakov equations in soliton theory.[22] The different signs of the second-order spatial derivatives in Eqs (28) and (29) result from the different dispersion [denoted by $\omega''(q)$] of the acoustic upper cutoff and the optical lower cutoff modes. At $q=\pi/a$, two cutoff modes have the same magnitude of dispersion but with different signs. For each envelope $A_j$, in addition to a self-modulation term $|A_j|^2A_j$, there is also a cross-phase modulation term $|A_j|^2A_{3-j}$ ($j=1,2$), which will drastically change the properties of the nonlinear localized excitations in comparison with the case of a single acoustic upper cutoff or a single optical lower cutoff mode if excited separately.

## 3 Coupled Soliton Solutions

### 3.1 *Single-Mode Excitations*

Let us first consider the single-mode excitations of Eqs (28) and (29). An optical lower cutoff mode excitation corresponds to $A_1=0$ but $A_2\neq 0$. Thus the Manakov equations (28) and (29) reduce to the nonlinear Schrödinger (NLS) equation for $A_2$,

$$\mathrm{i}\frac{\partial A_2}{\partial t}+\beta\frac{\partial^2 A_2}{\partial x_n^2}+P_2|A_2|^2A_2=0\,, \tag{35}$$

which, because $P_2>0$ and $\beta>0$, admits the soliton solution

$$A_2=\Big(\frac{2\beta}{P_2}\Big)^{1/2}k\,\mathrm{sech}\,[k(x_n-2kk_1\beta t)] \times\exp\{\mathrm{i}[k_1x_n-(k_1^2-k^2)\beta t]\} \tag{36}$$

with $k$ and $k_1$ two arbitrary constants. Thus for single-mode excitations it is ***impossible*** to obtain a kink for the optical lower cutoff mode.

The acoustic upper cutoff mode excitations correspond to setting $A_2=0$ but $A_1\neq 0$. Hence equations (28) and (29) are simplified to the NLS equation for $A_1$,

$$\mathrm{i}\frac{\partial A_1}{\partial t}-\beta\frac{\partial^2 A_1}{\partial x_n^2}+P_1|A_1|^2A_1=0\,, \tag{37}$$

which, depending on the sign of $P_1$, allows soliton and kink solutions. When $P_1>0$, we have the kink solution

$$A_1=\Big(\frac{2\beta}{P_1}\Big)^{1/2}k\tanh[k(x_n-2kk_1\beta t)] \times\exp\{\mathrm{i}[k_1x_n+(k_1^2+2k^2)\beta t]\}\,. \tag{38}$$

However, if $P_1<0$ one has the soliton solution

$$A_1=\Big(\frac{2\beta}{-P_1}\Big)^{1/2}k\,\mathrm{sech}\,[k(x_n-2kk_1\beta t)] \times\exp\{\mathrm{i}[k_1x_n-(k_1^2-k^2)\beta t]\}\,. \tag{39}$$

From the results obtained above, we have the conclusion that the optical lower cutoff mode is always a soliton but the acoustic upper cutoff mode may be either a soliton or a kink, depending on the parameters of the system. This picture, however, will be changed when the coupling of the two cutoff modes is taken into account.

### 3.2 *Coupled-Mode Excitations*

Now we turn our attention to the coupled nonlinear excitations of the system. This requires us to solve the coupled-mode equations (28) and (29) with $A_1$ and $A_2$ nonzero. We find that equations (28) and (29) admit the following coupled soliton solutions.

(i) ***Kink-soliton*** If $P_1P_2-Q_1Q_2>0$, $P_1+Q_2>0$ and $P_2+Q_1>0$, we have the coupled acoustic upper cutoff kink and optical lower cutoff soliton solution

$$A_1=W_1\tanh(kx_n+2\beta kk_1t)\exp[\mathrm{i}(k_1x_n-\Omega_1t)]\,, \tag{40}$$

$$A_2=W_2\,\mathrm{sech}\,(kx_n+2\beta kk_1t)\exp[\mathrm{i}(k_1x_n-\Omega_2t)] \tag{41}$$

with

$$W_1^2=\frac{2\beta k^2(P_2+Q_1)}{P_1P_2-Q_1Q_2}\,, \tag{42}$$

$$W_2^2=\frac{2\beta k^2(P_1+Q_2)}{P_1P_2-Q_1Q_2}\,, \tag{43}$$

$$\Omega_1=-\beta(2k^2+k_1^2)-\frac{2\beta k^2Q_1(P_1+Q_2)}{P_1P_2-Q_1Q_2}\,, \tag{44}$$

$$\Omega_2=\beta(k^2+k_1^2)-\frac{2\beta k^2P_2(P_1+Q_2)}{P_1P_2-Q_1Q_2}\,, \tag{45}$$

where $k$ and $k_1$ are two arbitrary constants. In this case the solution of Eqs (7) and (8) in the leading-order approximation takes the form

$$\phi_n(t)=W_1\tanh(kx_n+2\beta kk_1\beta t)(-1)^n\exp\{\mathrm{i}[k_1x_n-(\omega_1+\Omega_1)t]\} +\frac{S(J_2-J_1)}{\omega_2-\sigma_1}W_2\,\mathrm{sech}\,(kx_n+2\beta kk_1t)(-1)^n\exp\{\mathrm{i}[k_1x_n-(\omega_2+\Omega_2t)]\}\,, \tag{46}$$

$$\psi_n(t) = \frac{S(J_2 - J_1)}{\omega_1 - \sigma_2} W_1 \tanh(kx_n + 2\beta k k_1 \beta t)(-1)^n \exp\{\mathrm{i}[k_1 x_n - (\omega_1 + \Omega_1)t]\} + W_2 \,\mathrm{sech}\,(kx_n + 2\beta k k_1 t)(-1)^n \exp\{\mathrm{i}[k_1 x_n - (\omega_2 + \Omega_2 t)]\}\,. \tag{47}$$

If $k$ and $k_1$ are set to zero, the excitation denoted by Eqs (46) and (47) is a standing kink-soliton pair.

(ii) ***Soliton-kink*** If $P_1P_2 - Q_1Q_2 < 0$, $P_1 + Q_2 > 0$ and $P_2+Q_1 > 0$, one has the coupled acoustic upper cutoff soliton and optical lower cutoff kink solution

$$A_1 = W_1 \,\mathrm{sech}\,(kx_n + 2\beta k k_1 t) \exp[\mathrm{i}(k_1 x_n - \Omega_1 t)]\,, \tag{48}$$

$$A_2 = W_2 \tanh(kx_n + 2\beta k k_1 t) \exp[\mathrm{i}(k_1 x_n - \Omega_2 t)] \tag{49}$$

with

$$W_1^2 = \frac{2\beta k^2(P_2 + Q_1)}{P_1P_2 - Q_1Q_2}\,, \tag{50}$$

$$W_2^2 = \frac{2\beta k^2(P_1 + Q_2)}{P_1P_2 - Q_1Q_2}\,, \tag{51}$$

$$\Omega_1 = -\beta(2k^2 + k_1^2) - \frac{2\beta k^2 Q_1(P_1 + Q_2)}{P_1P_2 - Q_1Q_2}\,, \tag{52}$$

$$\Omega_2 = \beta(k^2 + k_1^2) - \frac{2\beta k^2 P_2(P_1 + Q_2)}{P_1P_2 - Q_1Q_2}\,, \tag{53}$$

where $k$ and $k_1$ are still two arbitrary constants. In this case the solution of Eqs (7) and (8) reads

$$\phi_n(t) = W_1 \,\mathrm{sech}\,(kx_n + 2\beta k k_1 \beta t)(-1)^n \exp\{\mathrm{i}[k_1 x_n - (\omega_1 + \Omega_1)t]\} + \frac{S(J_2 - J_1)}{\omega_2 - \sigma_1} W_2 \tanh(kx_n + 2\beta k k_1 t)(-1)^n \exp\{\mathrm{i}[k_1 x_n - (\omega_2 + \Omega_2 t)]\}\,, \tag{54}$$

$$\psi_n(t) = \frac{S(J_2 - J_1)}{\omega_1 - \sigma_2} W_1 \,\mathrm{sech}\,(kx_n + 2\beta k k_1 \beta t)(-1)^n \exp\{\mathrm{i}[k_1 x_n - (\omega_1 + \Omega_1)t]\} + W_2 \tanh(kx_n + 2\beta k k_1 t)(-1)^n \exp\{\mathrm{i}[k_1 x_n - (\omega_2 + \Omega_2 t)]\}\,. \tag{55}$$

When $k$ and $k_1$ are taken to be zero, equations (54) and (55) represent a standing soliton-kink pair.

From the results given above, we see that, different from the case of the single-mode excitation, the optical lower cutoff mode can be a kink due to the mode-mode coupling. The reason is that when the mode-coupling is taken into account, the cross-phase modulation can change the type of the nonlinear localized modes and hence result in the transition from soliton to kink, and vice versa.[23]

### 3.3 *Discussion for the Case $D_1 = D_2$*

The results presented in the last subsection showed that coupled soliton excitations are possible in the alternating Heisenberg ferromagnetic chain. One of the important properties is the frequency shift of relevant cutoff modes due to the nonlinear coupling. Such frequency shifts can be calculated from the formulae provided in Eqs (44) and (45) for the kink-soliton and Eqs (52) and (53) for the soliton-kink, respectively. Since too many parameters are involved, it is not easy to see the lowering or rising of their vibrating frequencies relative to the corresponding linear modes. Here for simplicity we assume $D_1 = D_2 = D$ to see the frequency shifts due to the nonlinear coupling.

Note that in this circumstance the coefficients of Eqs (28) and (29) take the values $\beta = J_1J_2Sa^2/[2(J_2 - J_1)] > 0$, $P_j = 4J_jS + 2(2S-1)D > 0$ $(j = 1, 2)$, $Q_2 = 4(2S-1)D > 0$ and $Q_1 = 4(2S-1)D - 2S(J_1 + J_2)$. Thus we always have positive $P_1 + Q_2$ and $P_2 + Q_1$. The results are given as follows.

(i) ***The kink-soliton case*** This type of coupled soliton [given by Eqs (40) and (41)] requires $P_1P_2 - Q_1Q_2 > 0$, which means $D > r$, where $r = T(1+\delta)(1+\rho)$ with $I = 2J_2S/[3(2S-1)]$, $\rho^2 = 1 + 3\delta/(1+\delta)^2$ and $\delta = J_1/J_2$. The vibrating frequency of the acoustic upper cutoff kink is $\omega_1 + \Omega_1$ [See the first term of Eqs (46) and (47)]. We obtain

(a) $\Omega_1 < 0$ if $y_1 < \beta_1$ and $D < r_1$;

(b) $\Omega_1 > 0$ if $1 < \beta_1 < y_1$ and $r_1 < D < r$;

where $\beta_1 = k_1^2/(2k^2)$ and

$$y_1 = \frac{\alpha_1^2 - \alpha_3}{2\rho\alpha_1 + \alpha_2}\,, \tag{56}$$

$$r_1 = \frac{I(1+\delta)}{\beta_1 - 1}\Big\{\beta_1 + \frac{1+5\delta}{4(1+\delta)} + \Big[\rho^2\beta_1^2 + \frac{\beta_1(1+2\delta)}{2(1+\delta)} + \frac{(7\delta-1)^2}{16(1+\delta)^2}\Big]^{1/2}\Big\} \tag{57}$$

with $\alpha_1 = \rho + (5+9\delta)/[4(1+\delta)]$, $\alpha_2 = (1+2\delta)/[2(1+\delta)]$ and $\alpha_3 = (7\delta-1)^2/[16(1+\delta)^2]$. From the case (a) we see that the vibrating frequency of the acoustic upper cutoff kink is in the acoustic band. The case (b) shows that in certain conditions, the vibrating frequency can also locate in the frequency gap between the acoustic and optical bands.

The vibrating frequency of the optical lower cutoff soliton is given by $\omega_2 + \Omega_2$. We find

(c) $\Omega_2 > 0$ when $\beta_1 < y_2$ and $D < r_2$;

(d) $\Omega_2 < 0$ if $\beta_1 > y_2$ and $r_2 < D < r$;

where

$$y_2 = \frac{f_3 - f_1^2}{2\rho f_1 + f_2}\,, \tag{58}$$

$$r_2 = \frac{I(1+\delta)}{3/2+\beta_1}\Big\{\beta_1 - \frac{1}{1+\delta} + \Big[\rho^2\beta_1^2 - \frac{(2-\delta)\beta_1}{(1+\delta)^2} + \frac{4-9\delta}{(1+\delta)^2}\Big]^{1/2}\Big\} \tag{59}$$

with $f_1 = 3(1+\rho)/2 + 1/(1+\delta)$, $f_2 = (2-\delta)/(1+\delta)^2$ and $f_3 = (4-9\delta)/(1+\delta)^2$. Thus the vibrating frequency of the optical lower cutoff soliton may be in and outside the frequency gap of the magnon bands.

(ii) ***The soliton-kink case*** The coupled soliton with this type requires $P_1P_2 - Q_1Q_2 < 0$, which means $D < r$. We find that, for any parameter of the system, $\Omega_1 < 0$, which yields the vibrating frequency of the acoustic upper cutoff soliton within the acoustic band. For the optical lower cutoff kink, we obtain

(e) $\Omega_2 > 0$ if $D < r_2$ and $\beta_1 > y_3$;

(f) $\Omega_2 < 0$ if $1 < \beta_1 < y_3$ and $r < D < r_3$.

Hence the vibrating frequency of the optical lower cutoff kink may be also in the band gap or in the optical band. This case is very different from the single-mode excitation, where the optical lower cutoff mode is always a soliton with its vibrating frequency in the gap.

## 4 Summary

Based on the quasi-discreteness multiple scale approach, we have investigated the dynamics of coupled gap solitons in the Heisenberg ferromagnetic chain with bond alternation. Nonlinear coupled-mode equations (i.e. the Manakov equations) have been derived for the envelopes of the acoustic upper cutoff and the optical lower cutoff modes. Coupled soliton-kink and kink-soliton solutions are provided explicitly. The results show that the vibrating frequencies of these nonlinearly coupled localized solitons can be within and outside the magnon spectrum band gap.

Band gap solitons have been observed experimentally in one-dimensional photonic crystals[24] and in the pendulum lattices.[25] Note that the alternating exchange interaction in magnetic systems can occur in layered materials of quasi-one-dimensional character[14] and other materials which may grow in a layered manner by molecular-beam epitaxy. Our results presented above for the coupled magnetic gap solitons may be useful for further understanding the excitation spectrum in magnetic systems and as a guide for new experimental findings.

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