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Intrinsic self-localized magnons in one-dimensional antiferromagnets

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The nonlinearity in magnon systems in one-dimensional Heisenberg antiferromagnets is shown to produce two types of intrinsic self-localized modes, symmetric and antisymmetric, below the magnon frequency band. In the case of extreme localization, the localized modes can be viewed as a two-spin bound state or a local spin-liquid state, where a pair of spins undergo a large excursion as compared with the rest of the spins.

Much attention has been focused recently on the low-lying energy spectra of one-dimensional (1D) antiferromagnets since Haldane conjectured that 1D Heisenberg antiferromagnets have a gap in the energy spectra for integral, but not for half-integral, spin values.[1] The conjecture has been tested by experiments in quasi-1D systems,[2-4] numerical calculations,[5] rigorous studies,[6] a stochastic geometrical approach,[7] and so on. In spite of much efforts, however, debates on the possible physical origin are still going on. Recently, a localized two-spin bound-state model has been presented by Date and Kindo[3] to interpret electron-spin-resonance (ESR) measurements of 1D antiferromagnets along the lines of Haldane's conjecture. Very recently, the present authors have shown the existence of an intrinsic, stationary self-localized mode below the magnon frequency band in d-dimensional antiferromagnets,[8] where a close conceptual analogy with intrinsic self-localized phonons in pure anharmonic crystal lattices[9] was exploited. This is a type of soliton mode, which may be viewed as a local spin-liquid state described by coherent states, where a cluster of spins undergo a large excursion while the rest of the spins undergo small-amplitude, plane-wave-like motion. Because of the indefiniteness of the magnon number involved in the localized mode, the degree of nonlinearity is presumed to be much higher than that of the usual, number-definite, two- and multiple-magnon bound modes.[10]

It is the purpose of this paper to study the properties of intrinsic self-localized magnons in 1D antiferromagnets, where the effect of the nonlinearity is the most pronounced of all the d-dimensional cases. It is shown that two types of stationary modes, symmetric and antisymmetric, characteristic of the 1D system, exist below the magnon frequency band.

The model spin Hamiltonian for 1D antiferromagnets that we study is given by

$$H=J\sum_i [\eta(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y)+S_i^zS_{i+1}^z],\ 0<\eta<1\ , \tag{1}$$

where S_i^α $(\alpha=x,y,z)$ is the α component of the spin operator S_i on the ith site in a 1D lattice, and the J and η are the nearest-neighbor exchange interaction constant and a constant characterizing the anisotropy, respectively. The effect of the uniaxial-anisotropic energy term will be studied later on. We assume that the 1D lattice is bipartite and divided into A and B sublattices, for which the Néel state is defined by $S^z=S$ and $-S$ where i is even and odd, respectively, where S is the magnitude of the spin operator. We introduce the Dyson-Maleev transformation[11,12]

$$S_i^+=(2S)^{1/2}[1-(a_i^\dagger a_i/2S)]a_i,\ S_i^-=(2S)^{1/2}a_i^\dagger,\ S_i^z=S-a_i^\dagger a_i \ \text{ for } i\in A\ , \tag{2a}$$

$$S_j^+=(2S)^{1/2}b_j^\dagger[1-(b_j^\dagger b_j/2S)],\ S_j^-=(2S)^{1/2}b_j,\ S_j^z=-S+b_j^\dagger b_j \ \text{ for } j\in B\ , \tag{2b}$$

to reduce Eq. (1) into the model boson Hamiltonian

$$H=2JS\left[\sum_i a_i^\dagger a_i+\sum_j b_i^\dagger b_i\right]+JS\eta\sum_{\langle ij\rangle}(a_i^\dagger b_j^\dagger+a_ib_j)-J\sum_{\langle ij\rangle}[(\eta/2)(a_i^\dagger a_i^2b_j+a_i^\dagger b_j^{\dagger 2}b_j)+a_i^\dagger b_j^\dagger a_ib_j]\ . \tag{3}$$

Here a_i $(a_i^\dagger)$ and b_j $(b_j^\dagger)$ are boson annihilation (creation) operators on the sublattices A and B, respectively, and the symbol $\sum_{\langle ij\rangle}$ denotes the sum over all nearest-neighbor pairs. The correspondence between the spin operators and the boson operators can be made exact by the introduction of a projection operator which projects out the unphysical boson states, i.e., the states where one or more lattice sites are each occupied by more than $2S$ bosons.[11] In what follows, we neglect such a projection operator, but the finite-ladder structure of the eigenstate of the spin operator will be taken care of at a later stage.

We are concerned with solitonlike intrinsic self-localized modes induced by the nonlinearity in the magnon system in Eq. (3), in which a cluster of spins undergo a large excursion as compared with the rest of the spins. A physically acceptable candidate for quantum states of such large-amplitude collective modes may be coherent states.[13] We therefore employ the coherent-state ansatz for the eigenfunction $\Psi(t)$ of H,

$$\Psi(t)=\prod_n \exp[-(\tfrac{1}{2})(|\alpha_n|^2+|\beta_n|^2)] \times\exp(\alpha_n a_n^\dagger+\beta_n b_n^\dagger)|0\rangle\,, \quad (4)$$

where $|0\rangle$ is the vacuum state of the boson system, and then we set up the time-dependent variational principle[13]

$$\delta\int dt\langle\Psi(t)|i\hbar(\partial/\partial t)-H|\Psi(t)\rangle=0\,. \quad (5)$$

In Eq. (4), the index n denotes the position of the unit cell in the 1D lattice, and $\alpha_n\equiv\alpha_n(t)$ and $\beta_n\equiv\beta_n(t)$ and their complex conjugates α_n^* and β_n^* are c-number functions of n and t. The coherent-state representation $\langle\Psi(t)|H|\Psi(t)\rangle$ of H in Eq. (5) is identical to Eq. (3) with a_n, $a_n^\dagger$, b_n, and $b_n^\dagger$ replaced by α_n, α_n^*, β_n, and β_n^*, respectively, for all n. Then the variational principle yields (hereafter we use units with $\hbar=1$)

$$i(d\alpha_n/dt)=(\partial/\partial\alpha_n^*)\langle\Psi(t)|H|\Psi(t)\rangle$$
$$=2JS\alpha_n+JS\eta(\beta_n^*+\beta_{n-1}^*)-J\{(\eta/2)[\alpha_n^2(\beta_n+\beta_{n-1})+|\beta_n|^2\beta_n^*+|\beta_{n-1}|^2\beta_{n-1}^*]+\alpha_n(|\beta_n|^2+|\beta_{n-1}|^2)\}\,, \quad (6a)$$

$$-(d\beta_n^*/dt)=(\partial/\partial\beta_n)\langle\Psi(t)|H|\Psi(t)\rangle$$
$$=2JS\beta_n^*+JS\eta(\alpha_n+\alpha_{n+1})-J\{(\eta/2)[\beta_n^{*2}(\alpha_n^*+\alpha_{n+1}^*)+|\alpha_n|^2\alpha_n+|\alpha_{n+1}|^2\alpha_{n+1}]+\beta_n^*(|\alpha_n|^2+|\alpha_{n+1}|^2)\}\,. \quad (6b)$$

In Eqs. (6), the nonlinearity in the magnon system is fully taken into account, though they are a classical analog of the corresponding q-number equation.

We seek stationary-mode solutions to Eqs. (6) by setting

$$\alpha_n=u_n\exp(-i\omega t),\quad \beta_n^*=v_n\exp(-i\omega t)\,, \quad (7)$$

where u_n and v_n are real functions of n and independent of t. Inserting Eqs. (7) into Eqs. (6), we get

$$2JSu_n+JS\eta(v_n+v_{n-1})-(J/2)F_1(u_n,v_n)=\omega u_n\,, \quad (8a)$$

$$2JSv_n+JS\eta(u_n+u_{n+1})-(J/2)F_2(u_n,v_n)=-\omega v_n\,, \quad (8b)$$

where

$$F_1(u_n,v_n)=\eta[u_n^2(v_n+v_{n-1})+v_n^3+v_{n-1}^3] +2u_n(v_n^2+v_{n-1}^2)\,, \quad (9a)$$

$$F_2(u_n,v_n)=\eta[v_n^2(u_n+u_{n+1})+u_n^3+u_{n+1}^3] +2v_n(u_n^2+u_{n+1}^2)\,. \quad (9b)$$

We pay attention to ω lying below the bottom $\omega_m=2JS(1-\eta^2)^{1/2}$ of the magnon frequency band

$$\omega(k)=2JS[1-\eta^2\cos^2(ka)]^{1/2}\,, \quad (10)$$

where k and a are a wave vector and the distance of the nearest-neighbor spins, respectively. In terms of a 2×2 lattice Green's-function matrix

$$G(n)\equiv G(n,\omega)=(G_{\mu\nu}(n))\equiv(G_{\mu\nu}(n,\omega)),\quad \mu,\nu=1,2\,, \quad (11)$$

$$G_{\mu\nu}(n,\omega)=\frac{1}{N}\sum_k b_{\mu\nu}(k)\exp(2ikna)/[\omega(k)^2-\omega^2]\,, \quad (12)$$

where

$$b_{11}(k)=2JS+\omega,\quad b_{22}(k)=2JS-\omega\,,$$
$$b_{12}(k)=-JS\eta(1+e^{-2ika}),\quad b_{21}=-JS\eta(1+e^{2ika})\,, \quad (13)$$

Eqs. (8) are rewritten as

$$u_n=\frac{J}{2}\sum_m[G_{11}(n-m)F_1(u_m,v_m) +G_{12}(n-m)F_2(u_m,v_m)]\,, \quad (14a)$$

$$v_n=\frac{J}{2}\sum_m[G_{21}(n-m)F_1(u_m,v_m) +G_{22}(n-m)F_2(u_m,v_m)]\,. \quad (14b)$$

In Eqs. (14) the sums extend over the first Brillouin zone, and N is the total number of unit cells in the 1D lattice. For ω lying outside the magnon frequency band $\omega(k)$, $G_{\mu\nu}(n,\omega)$ is a rapidly (exponentially) decreasing function of $|n|$. Therefore, we need only consider Eqs. (14) associated with the central position of the localized mode and its neighbors.

As an illustration, let us consider a one-localized-mode problem that a stationary self-localized mode is located at an $n=0$ unit-cell site. Here, two types of the localized mode of physical interest having the symmetry

$$u_{-n}(-\omega)=\pm v_n(\omega),\quad v_{-n}(-\omega)=\pm u_n(\omega) \quad (15)$$

are shown to exist (see Fig. 1). The modes with plus and minus signs on the right-hand side are referred to as a

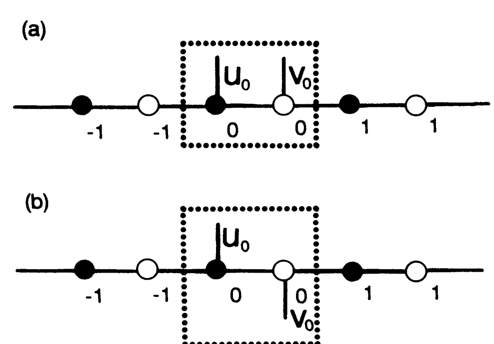

FIG. 1. Profile functions u_0 and v_0 at the central position $n=0$ of a self-localized mode. (a) Symmetric mode and (b) antisymmetric mode.

symmetric mode (SM) and an antisymmetric mode (AM), respectively. Let us set

$$u_n = A\xi_n,\ v_n = A\zeta_n\ , \tag{16}$$

$$\xi_0 = \zeta_0 = 1 \text{ for SM},\ \xi_0 = -\zeta_0 = 1 \text{ for AM}. \tag{17}$$

Then the quantities ξ_n and ζ_n are reduced profile functions of the localized mode, and A is identified as its amplitude. Inserting Eqs. (16) into Eqs. (14) and using identity relations satisfied by the $G_{\mu\nu}(n,\omega)$'s and Eqs. (15) and (17), we obtain an exact formal expression for the eigenfrequency ω of the localized mode in terms of ξ_1:

$$\omega = 2JS[1 \pm (\eta/2)(1+\xi_1) \mp (\lambda\eta/2)(2+\xi_1+\xi_1^3) - \lambda(1+\xi_1^2)]\ , \tag{18}$$

where

$$\lambda = A^2/2S = |\alpha_0|^2/2S = |\beta_0|^2/2S < 1\ . \tag{19}$$

Here the condition $\lambda < 1$ has been imposed to take into account the finite-ladder structure of the spin state.[11]

To understand the physical properties of the self-localized modes, we are concerned here with obtaining an approximate analytical expression for ξ_1 rather than its numerical value. This can be done by limiting our discussion to the mode lying far below the magnon frequency band in comparison with the magnon bandwidth, i.e.,

$$\bar{\omega}^2 \equiv (\omega/2JS)^2 \ll 1,\ \eta^2 \ll 1\ , \tag{20}$$

where the localized mode is spatially well localized, satisfying the relation $1 \gg \xi_1,\ \zeta_1 \gg \xi_2, \zeta_2, \ldots$. Then, inserting Eqs. (16) into Eqs. (14), using (20) and also asymptotic analytical expressions for the $G_{\mu\nu}(n,\omega)$'s for small $\bar{\omega}$, we obtain after lengthy, though straightforward, calculations

$$\xi_1 = -\lambda\eta^2/2(1-\lambda) \ll 1\ . \tag{21}$$

Combining Eq. (21) with Eq. (18) leads to

$$\omega = 2JS[1 \pm (\eta/2) - \lambda(1 \pm \eta)] < 2JS(1-\eta^2)^{1/2}\ , \tag{22}$$

with $2\lambda > \eta$ for SM and $2\lambda > -\eta$ for AM.

We are now in a position to include the uniaxial-anisotropy energy term in Eq. (1):

$$H = J\sum_i [\eta(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + S_i^z S_{i+1}^z] - D\sum_i (S_i^z)^2\ , \tag{23}$$

where D is the uniaxial-anisotropy energy constant. Let us consider its effect on Eqs. (8). It is shown that it simply introduces the following modifications $2JS \to 2JS + (2S-1)D$, $F_1(u_n,v_n) \to F_1(u_n,v_n) + (4D/J)u_n^3$, and $F_2(u_n,v_n) \to F_2(u_n,v_n) + (4D/J)v_n^3$. Correspondingly, the quantities ξ_1 and ω in Eqs. (21) and (22) are modified to

$$\xi_1 = -\lambda\eta(\eta-\bar{D})/2(1+\bar{D}-\lambda)(1+\bar{D})\ , \tag{24}$$

$$\omega = 2JS[1+\bar{D}-2\lambda\bar{D} \pm (\eta/2) - \lambda(1 \pm \eta)] < \omega_m\ , \tag{25}$$

with

$$\bar{D} = (2S-1)D/2JS,\ \omega_m = 2JS[(1+\bar{D})^2 - \eta^2]^{1/2}\ . \tag{26}$$

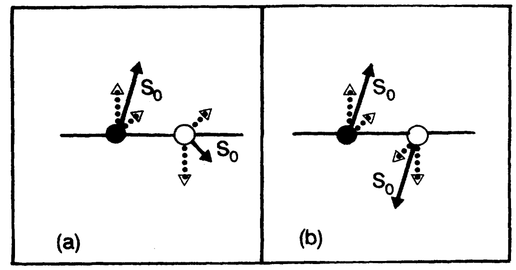

FIG. 2. Schematic feature of the spin configuration of a self-localized mode or a two-spin bound mode. (a) Symmetric mode and (b) antisymmetric mode.

It is seen that for $D > 0$, the essential feature of the properties of the self-localized modes remain unchanged by the inclusion of D.

A characteristic feature of the self-localized modes here is that both of the symmetric and antisymmetric modes are strongly localized provided inequalities (20) hold. Actually, this is a two-spin bound state appearing below the magnon frequency band, in which a pair of the spins undergo a large excursion, while the rest of the spins undergo small-amplitude wavelike motion. The intrinsic self-localized modes, which are described by coherent states, may therefore be regarded as a local spin-liquid state. A schematic feature of the symmetric mode and the antisymmetric mode are depicted in Fig. 2, and their frequency-level diagram is shown in Fig. 3, taking the case $\eta = \frac{1}{2}$, $\lambda = \frac{1}{3}$, and $D = 0$ as an illustrative example.

In this paper we have developed a theory of self-localized modes in 1D antiferromagnets by applying the Dyson-Maleev transformation[11,12] and the variational procedure in the coherent-state representation.[13] By its nature, such a formulation can be used at least for $S \gg 1$. From the obtained result, we may conclude that low-lying energy states of the 1D antiferromagnets are significantly different from that given by the conventional spin-wave theory. Here, the self-localized mode having the character of an envelope soliton in a lattice space may also be

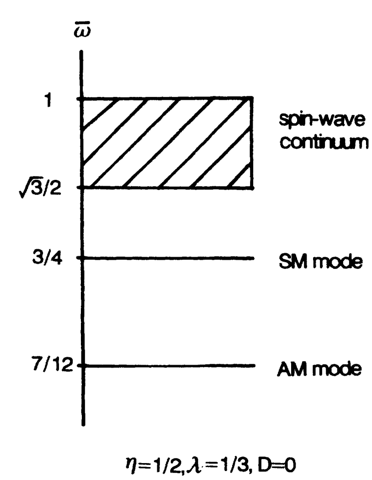

FIG. 3. Graphical illustration of the frequency level of self-localized modes for $\eta = \frac{1}{2}$, $\lambda = \frac{1}{3}$, and $D = 0$.

viewed as a local spin-liquid state in which a large local spin deviation exists as compared with the rest of the system. Such a nonlinear mode can be considered as a nontopolotical soliton, while intrinsic defects considered by Haldane[14] and an instanton discussed by Balakrishnan, Bishop, and Dandoloff[15] for classical continuous 1D antiferromagnets can be considered as topological ones. For such topological solitons, discussions have been given on the difference of the Berry phase[16] for odd- and even-integer S and its implication on the ground-state properties of antiferromagnets.[1,14] On the other hand, the method employed here is obviously not sensitive to the parity problem, though the obtained result is conceptually similar to the two-spin bound-state model of the Haldane problem[1] by Date and Kindo.[3] In this sense, much remains to be done to see whether or not the low-lying state associated with the stationary localized magnon mode is directly responsible for the Haldane state.

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