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Solitary Magnon Localization in Antiferromagnet $Ni(C_2H_8N_2)_2NO_2ClO_4$

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Employing the Holstein-Primakoff transformation and the coherent state ansatz, we obtain two partial differential equations of motion from Hamiltonian. Using the method of multiple scalar, we reduce these equations into a nonlinear Schrodinger equation and get the single soliton solution. These results show that solitary magnon localization in antiferromagnet $Ni(C_2H_8N_2)_2NO_2ClO_4$ is possible.

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$Ni(C_2H_8N_2)_2NO_2ClO_4$ (NENP) is the best real system approaching the ideal linear-chain Heisenberg antiferromagnet[1] (AFM). The pure NENP single crystal has a structure of orthorhombic system defined with orthogonal axis $(a, c, b) \equiv (x, y, z)$.[2] The magnetic chains are made of Ni^{2+} ions disposed along the b axis. The single-ion anisotropy and the interchain exchange interaction are both small compared to the interchain exchange interaction. The optical resonance transitions between the ground state and the first excited states give directly evidence for the Haldane gap.

The Hamiltonian describing AFM NENP under the external magnetic field $\boldsymbol{H}_{ex}$ is

$$H = \sum_{ij} \{J\boldsymbol{S}_i \cdot \boldsymbol{S}_j + D(S_i^z)^2 + E[(S_i^x)^2 - (S_i^y)^2] - g\mu_B \boldsymbol{H}_{ex} \cdot \boldsymbol{S}_i\} , \tag{1}$$

where J is the intrachain exchange parameter, D and E are longitudinal single-ion and in-plane anisotropy, g is the Lande factor and μ_B is the Bohr magneton.

The AFM NENP is divided into two interpenetrating sublattices A and B. Introducing the Holstein-Primakoff transformation

$$S_i^+ = (2S - a_i^+ a_i)^{\frac{1}{2}} a_i^- , \quad S_i^- = a_i^+ (2S - a_i^+ a_i)^{\frac{1}{2}} , \quad S_i^z = S - a_i^+ a_i , \quad \text{for } i \in \text{A and}$$
$$S_j^+ = b_j^+ (2S - b_j^+ b_j)^{\frac{1}{2}} , \quad S_j^- = (2S - b_j^+ b_j)^{\frac{1}{2}} b_j , \quad S_j^z = b_j^+ b_j - S , \quad \text{for } j \in \text{B (Ref. 3)} ,$$

we get boson Hamiltonian

$$\begin{aligned} H = \sum_{(ij)} J[&\frac{1}{2}(2S - a_i^+ a_i)^{\frac{1}{2}} a_i (2S - b_j^+ b_j)^{\frac{1}{2}} b_j + \frac{1}{2} a_i^+ (2S - a_i^+ a_i)^{\frac{1}{2}} b_j^+ (2S - b_j^+ b_j)^{\frac{1}{2}} \\ &- (S - a_i^+ a_i)(b_j^+ b_j - S)] + \sum_i [D(S - a_i^+ a_i)^2 + \frac{1}{2} E(2S - a_i^+ a_i) a_i^2 \\ &+ \frac{1}{2} E a_i^{+2} (2S - a_i^+ a_i) - g\mu_B H_{ex}^z (S - a_i^+ a_i)] + \sum_j [D(b_i^+ b_i - S)^2 \\ &+ \frac{1}{2} E b_i^{+2} (2S - b_i^+ b_j) + \frac{1}{2} E(2S - b_j^+ b_j) b_j^2 - g\mu_B H_{ex}^z (b_j^+ b_j - S)] , \end{aligned} \tag{2}$$

where $a_i(a_i^+)$ and $b_j(b_j^+)$ are annihilation (creation) operator associated with the A and B sublattices, S is the magnitude of the spin operators.

As far as the solitary excitations induced by magnon-magnon interactions are concerned, a physically acceptable candidate for quantum state is coherent state. We therefore employ the coherent state ansatz for the eigenstates

$$\Psi(t) = \exp[-\frac{1}{2}(\sum_i |\alpha_i(t)|^2 + \sum_j |\beta_j(t)|^2)] \exp[\sum_i \alpha_i(t) a_i^+ + \sum_j \beta_j(t) b_j^+]|0\rangle$$

of H and set up the time-dependent variational principle:[4]

$$\delta \int dt \langle \Psi(t)| i\hbar \frac{\partial}{\partial t} - H|\Psi(t)\rangle = 0 . \tag{3}$$

The coherent state representation $\langle \Psi(t)|H|\Psi(t)\rangle$ of H in Eq. (3) is identical to Eq. (2) with $a_i(a_i^+)$, $b_j(b_j^+)$ replaced by $\alpha_i(\alpha_i^*)$, $\beta_j(\beta_j^*)$ for all i and j. Then the variational principle yields the equations of motion for the α_i's β_j's:

$$\begin{aligned} i\hbar\frac{d\alpha_i}{dt} =& [2S(E-D) + g\mu_B H_{ex}^z]\alpha_i + S(\beta_j^* + \beta_{j-1}^*) + (2D\alpha_i - \frac{3}{2}E\alpha_i^*)|\alpha_i|^2 - \frac{1}{2}E\alpha_i^3 \\ & - \frac{1}{4}\alpha_i^2(\beta_j + \beta_{j-1}) - \frac{1}{4}(|\beta_j|^2\beta_j^* + |\beta_{j-1}|^2\beta_{j-1}^*) - \frac{1}{2}|\alpha_i|^2(\beta_j^* + \beta_{j-1}^*) \\ & + \frac{1}{16S}\alpha_i^2(|\beta_j|^2\beta_j + |\beta_{j-1}|^2\beta_{j-1}) - \frac{1}{16S}|\alpha_i|^2\alpha_i^2(\beta_j + \beta_{j-1}) - \frac{3}{32S}|\alpha_i|^4(\beta_j^* + \beta_{j-1}^*) \\ & + \frac{1}{8S}|\alpha_i|^2(|\beta_j|^2\beta_j^* + |\beta_{j-1}|^2\beta_{j-1}^*) - \frac{1}{32S}(|\beta_j|^4\beta_j^* + |\beta_{j-1}|^4\beta_{j-1}^*) , \end{aligned} \tag{4}$$

$$\begin{aligned} i\hbar\frac{d\beta_j}{dt} =& [2S(E-D) - g\mu_B H_{ex}^z]\beta_j + S(\alpha_i^* + \alpha_{i+1}^*) + (2D\beta_j - \frac{3}{2}E\beta_j^*)|\beta_j|^2 - \frac{1}{2}E\beta_j^3 \\ & - \frac{1}{4}\beta_j^2(\alpha_i + \alpha_{i+1}) - \frac{1}{4}(|\alpha_i|^2\alpha_i + |\alpha_{i+1}|^2\alpha_{i+1}) - \frac{1}{2}|\beta_j|^2(\alpha_i^* + \alpha_{i+1}^*) \\ & + \frac{1}{16S}\beta_j^2(|\alpha_i|^2\alpha_i + |\alpha_{i+1}|^2\alpha_{i+1}) - \frac{1}{16S}|\beta_j|^2\beta_j^2(\alpha_i + \alpha_{i+1}) - \frac{3}{32S}|\beta_j|^4(\alpha_i^* + \alpha_{i+1}^*) \\ & + \frac{1}{8S}|\beta_j|^2(|\alpha_i|^2\alpha_i^* + |\alpha_{i+1}|^2\alpha_{i+1}^*) - \frac{1}{32S}(|\alpha_j|^4\alpha_i^* + |\alpha_{i+1}|^4\alpha_{i+1}^*) , \end{aligned} \tag{5}$$

Eqs. (4) and (5) involve terms up to the fifth order in $\alpha_i(\alpha_i^*)$, $\beta_j(\beta_j^*)$. Although Eqs. (4) and (5) are transformed into the c-number equations, it is very difficult to solve them because of the nonlinearity and discreteness. The AFM NENP is divided into two sublattices A and B with lattice constant $2d_0$, a typical wavelength of excitations λ_0 is assumed $\lambda_0 >> 2d_0$, then we may take the continuum approximation

$$\alpha_i(t) \to \Psi_1(x,t) , \quad \alpha_{i\pm1}(t) \to \Psi_1 \pm \eta\Psi_{1x} \pm \frac{1}{2!}\eta^2\Psi_{1xx} \pm \frac{1}{3!}\eta^3\Psi_{1xxx} \pm O(\eta^4) \text{ and}$$

$$\beta_j(t) \to \Psi_2(x,t) , \quad \beta_{j\pm1}(t) \to \Psi_2 \pm \eta\Psi_{2x} \pm \frac{1}{2!}\eta^2\Psi_{2xx} \pm \frac{1}{3!}\eta^3\Psi_{2xxx} \pm O(\eta^4) ,$$

where $\eta = 2d_0/\lambda_0$ is a small dimensionless parameter. In this paper, we only consider the case

$O(\eta^2)$. Retaining terms in Eqs. (4) and (5) to $O(\eta^2)$, we have

$$\begin{aligned} i\hbar\Psi_{1t} =&[2S(E-D)+g\mu_B H_{ex}^z]\Psi_1+S(2\Psi_1^*-\eta\Psi_{2x}^*+\frac{1}{2}\eta^2\Psi_{2xx}^*)+2D\Psi_1|\Psi_1|^2 \\ &-\frac{3}{2}E\Psi_1^*|\Psi_1|^2-\frac{1}{4}\Psi_1^2(2\Psi_2-\eta\Psi_{2x}+\frac{1}{2}\eta^2\Psi_{2xx})-\frac{1}{2}|\Psi_1|^2(2\Psi_2^*-\eta\Psi_{2x}^*+\frac{1}{2}\eta^2\Psi_{2xx}^*) \\ &-\frac{1}{2}E\Psi_1^3-\frac{1}{4}[\Psi_2^*|\Psi_2|^2+(\Psi_2^*-\eta\Psi_{2x}^*+\frac{1}{2}\eta^2\Psi_{2xx}^*)|\Psi_2-\eta\Psi_{2x}+\frac{1}{2}\eta^2\Psi_{2xx}|^2], \end{aligned} \tag{6}$$

$$\begin{aligned} i\hbar\Psi_{2t} =&[2S(E-D)+g\mu_B H_{ex}^z]\Psi_2+S(2\Psi_1^*+\eta\Psi_{1x}^*+\frac{1}{2}\eta^2\Psi_{1xx}^*)+2D\Psi_2|\Psi_2|^2 \\ &-\frac{3}{2}E\Psi_2^*|\Psi_2|^2-\frac{1}{4}\Psi_2^2(2\Psi_1+\eta\Psi_{1x}+\frac{1}{2}\eta^2\Psi_{1xx})-\frac{1}{2}|\Psi_2|^2(2\Psi_1^*+\eta\Psi_{1x}^*+\frac{1}{2}\eta^2\Psi_{1xx}^*) \\ &-\frac{1}{2}E\Psi_2^3-\frac{1}{4}[\Psi_1^*|\Psi_1|^2+(\Psi_1^*+\eta\Psi_{1x}^*+\frac{1}{2}\eta^2\Psi_{1xx}^*)|\Psi_1+\eta\Psi_{1x}+\frac{1}{2}\eta^2\Psi_{1xx}|^2]. \end{aligned} \tag{7}$$

We use the method of multiple scalar to reduce Eqs. (6) and (7) into another nonlinear equation which can be solved exactly.[5] This technique calls for the introduction of different spatial scales $x_j=\mu^j x$ and time scales $t_j=\mu^j t$ ($\mu<<1$, $j=0,1,2,\cdots$). Then the first spatial and temporal derivatives are written as expansions:

$$\frac{\partial}{\partial t}=\frac{\partial}{\partial t_0}+\mu\frac{\partial}{\partial t_1}+\mu^2\frac{\partial}{\partial t_2}+\cdots, \quad \frac{\partial}{\partial x}=\frac{\partial}{\partial x_0}+\mu\frac{\partial}{\partial x_1}+\mu^2\frac{\partial}{\partial x_2}+\cdots,$$

from which expressions for higher derivatives follow straightforwardly. Similarly, the quantities Ψ_1 and Ψ_2 are also written as

$$\Psi_1=\mu\Psi_1^{(1)}+\mu^2\Psi_1^{(2)}+\cdots, \quad \Psi_2=\mu\Psi_2^{(1)}+\mu^2\Psi_2^{(2)}+\cdots,$$

where $\Psi_1^{(j)}$ and $\Psi_2^{(j)}$ are functions of all x_j and t_j ($j=1,2,3,\cdots$), but these arguments will not be written explicitly. These expansions above are now substituted into Eqs. (6) and (7), terms with equal powers of μ are collected, we obtain the equations for $\Psi_1^{(3)}$, $\Psi_2^{(3)}$ as follows:

$$\begin{aligned} &[(i\hbar\frac{\partial}{\partial t_0}-\omega_1)(i\hbar\frac{\partial}{\partial t_0}-\omega_2)-L_1L_2]\Psi_1^{(3)} \\ &=(\omega_1+\omega_2-2\omega)[i\hbar\frac{\partial A}{\partial t_2}+\frac{1}{2}\omega''(k)\frac{\partial^2 A}{\partial\xi^2}+\lambda|A|^2A]\exp[i(kx_0-\omega t_0)], \end{aligned} \tag{8}$$

$$(i\hbar\frac{\partial}{\partial t_0}-\omega_2)\Psi_2^{(3)}-L_2\Psi_1^{(3)*}=\beta_2^{(3)}, \tag{9}$$

where $\xi=\mu(x-c_g t)$, λ is a parameter to be determined. The terms proportional to $\exp[i(kx_0-\omega t_0)]$ are secular terms,[5] then we demand the coefficient of $\exp[i(kx_0-\omega t_0)]$ be zero in order to apply the perturbation theory. This forces function A to satisfy $i\hbar\partial A/\partial t_2+\omega''(k)\partial^2 A/2\partial\xi^2+\lambda|A|^2A=0$. This is the nonlinear Schrodinger equation.[5] The single soliton solution is written as

$$A=(\frac{Sc_1^2\omega''(k)}{\lambda\mu^2})^{\frac{1}{2}}\mathrm{sech}\{c_1[x-(c_g+c_2\omega''(k))t-x_0]\}\exp\{i[(k+c_2)x-\Omega t-\Phi_0]\}, \tag{10}$$

$$\Omega=\omega+c_g c_2+\frac{1}{2}(c_2^2-c_1^2)\omega''(k), \tag{11}$$

where c_1, c_2, x_0 and ϕ_0 are integration constants. Equation (10) is a wave packet traveling to the right with velocity $c_g + c_2\omega''(k)$. If c_2 is set to be zero, Eq. (11) becomes $\Omega = \omega - c_1^2\omega''(k)/2$ at $k = 0$ or $\pi/2d_0$ ($c_g = 0$). For the "acoustic branch" and the "optical branch", the soliton frequencies have four values:

$$\Omega_{\max}(k=0) = \omega_{\max} - \frac{1}{2}c_0^2\omega''_{\max} > \omega_{\max}\ , \quad \Omega_{-\max}(k=\frac{\pi}{2d}) = \omega_{-\max} - \frac{1}{2}c_0^2\omega''_{-\max} > \omega_{-\max}\ ,$$

$$\Omega_{\min}(k=\frac{\pi}{2d}) = \omega_{\min} - \frac{1}{2}c_0^2\omega''_{\min} < \omega_{\min}\ , \quad \Omega_{-\min}(k=0) = \omega_{-\min} - \frac{1}{2}c_0^2\omega''_{-\min} < \omega_{-\min}\ .$$

These soliton frequencies enter into the frequency gap of the linear dispersion relation and denote the solitary localized modes in the AFM NENP.

The spatial configuration of the spin for the single soliton case is given by

$$\langle S_i^z\rangle \to S - \frac{Sc_1^2\omega''(k)}{\lambda}\mathrm{sech}^2\{\{c_1\{x - [\omega'(k) + c_2\omega''(k)]t - x_0\}\}\}\ , \tag{12}$$

$$\langle S_j^z\rangle \to S - \frac{S^3c_1^2J^2(4+K^2d^2)}{4\lambda(\omega-\omega_2)^2}\mathrm{sech}^2\{\{c_1\{x - [\omega'(k) + c_2\omega''(k)]t - x_0\}\}\}\ . \tag{13}$$

Equations (12) and (13) show analytically the magnon localization in AFM NENP. They are typical solitary excitations in NENP.

How treat the consistent problems of solitary excitations in the FM chain by using the coherent state method? These arguments have not been settled. Skrinjar *et al.*[6] thought that it is impossible to establish a direct relation between ε and λ_0. They have not found the good method to avoid the inconsistence of the two-parameter theory of solitons in magnetic systems. For studying the solitary excitations in FM and AFM, our approach is consistent and systematic. This approach is a good method in investigating solitary excitations of the FM and AFM.

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