Solitons with Internal Degrees of Freedom in 1D Heisenberg Antiferromagnets

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The dynamics and statistical mechanics of two-parametric solitons (dyons) in a weakly nonuniaxial Heisenberg antiferromagnetic chain are considered. The dyon contribution to the dynamic structure factor is calculated, and resonance frequencies for the recently studied 1D antiferromagnet $CsMnI_3$ are estimated.

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It is well known that solitons play an important role in the physics of one-dimensional (1D) systems, being a separate type of elementary excitation [1,2]. Magnetic chains in solids are a good realization of 1D systems, and soliton signatures were reliably observed in static and dynamic characteristics of various 1D magnets with both ferro- and antiferromagnetic coupling [3]. Topologically nontrivial soliton excitations, apart from being movable defects in magnetic order, can possess additional internal degrees of freedom, such as magnon modes localized at a kink [4], or precession of spins inside a kink [5,6]; such solitons with extra degrees of freedom are usually called dyons [7]. In 1D antiferromagnets (AFM's) they are responsible for subtle quantum effects distinguishing between spin chains with integer and half-integer spin [6,7]. Characteristic frequencies of the internal motion can be detected in principle by electron spin resonance (ESR) or inelastic neutron scattering (INS). In three dimensions, magnon modes localized at the domain walls in AFM's were experimentally observed in thulium orthoferrite [8]. In one dimension, dyon signatures were observed in the Ising-type quasi-1D AFM $CsCoCl_3$ in ESR and INS experiments as the so-called "soliton magnetic resonance" [9]. For Heisenberg magnets, to the knowledge of the authors, there are no observations of effects which could be attributed to dyons.

This Letter is devoted to internal kink modes in 1D (classical) Heisenberg antiferromagnets. We consider a continuum model of an easy-axis antiferromagnetic chain with weak biaxial (orthorhombic) anisotropy, and show that in the case of the AFM even in a classical model with sufficiently large spin value (e.g., $S = 5/2$), internal kink modes have quantum features absent in ferromagnets (FM's). A kink in an AFM acts as a nonlinear periodic potential for the dynamics of localized modes, with strong quantum tunneling between wells. Taking that into account, we construct a dyon phenomenology for the statistical mechanics of a soliton gas, in the spirit of Ref. [2]. Further, we calculate the dyon contribution to the dynamic structure factor (DSF), and apply the results to predict resonance frequencies for the recently studied quasi-1D AFM compound $CsMnI_3$ [10,11].

The model.—Consider the classical model of a Heisenberg easy-axis AFM with rhombic anisotropy which can be described by the following Hamiltonian:

$$H = \sum_i \{J\vec{S}_i \cdot \vec{S}_{i+1} + D_1(S_i^x)^2 + D_2(S_i^y)^2\}. \quad (1)$$

Here $J > 0$ is the exchange constant, $D_{1,2}$ are anisotropy constants, and spins $\vec{S}_i$ are treated as classical vectors of length S, situated at the sites of a one-dimensional lattice with lattice constant a. We assume that $D_1 > D_2 > 0$, then z is the easy axis, and (zy) is the easiest plane. It is convenient to introduce the rhombicity parameter $\rho = (D_1/D_2) - 1$; in purely uniaxial AFM's $\rho = 0$, and $\rho \gg 1$ corresponds to the almost easy-plane situation. This model is sufficiently simple from the theoretical point of view and, besides that, can describe several real quasi-1D magnets. For example, $CsMnI_3$ is well described by the Hamiltonian (1) with $\rho \simeq 0$ [11], and for CMC ($CsMnCl_3 \cdot 2H_2O$) $\rho \simeq 3$ [12].

Dynamics.—A low-energy, continuum model of AFM's can be derived in the usual way [13]. We define normalized vectors of magnetization $\vec{m}_n$ and vectors of antiferromagnetism $\vec{l}_n$ as linear combinations of spins in pairs of neighboring lattice sites: $\vec{m}_n = (\vec{S}_{2n} + \vec{S}_{2n+1})/2S$, $\vec{l}_n = (\vec{S}_{2n} - \vec{S}_{2n+1})/2S$. Vectors $\vec{m}$ and $\vec{l}$ are defined on a lattice with the spacing $2a$ and are subjected to the constraints $\vec{m} \cdot \vec{l} = 0$, $\vec{l}^2 + \vec{m}^2 = 1$. This procedure of breaking the original lattice into dimers is necessary to keep the total number of degrees of freedom unchanged. For low temperatures and weak magnetic fields the magnetization in AFM is small, $|\vec{m}| \ll |\vec{l}|$. Taking that into account, one can pass to the continuum limit and introduce the Lagrangian via $L = \int (dx/a) S\hbar\vec{m}(\vec{l} \times \partial\vec{l}/\partial t) - H$ (see Ref. [14]; the integrand in the first term in L is nothing but Berry's phase [15] for a spin dimer). Note that H contains a parity-breaking term proportional to $\vec{m}\nabla\vec{l}$ which is a consequence of the translational noninvariance of breaking the lattice into dimers when passing to the continuum limit.

After integrating out the degrees of freedom corresponding to $\vec{m}$, one obtains an effective Lagrangian depending on $\vec{l}$ only, where $\vec{l}$ now has to be considered as a unit vector $\vec{l}^2 \simeq 1$. The effective Lagrangian density $\mathcal{L}$ can be written in the form of the anisotropic σ model with a topological term [13]:

$$\mathcal{L} = (1/2)JS^2a\{c^{-2}(\partial\vec{l}/\partial t)^2 - (\nabla\vec{l})^2 - x_{01}^{-2}l_x^2 - x_{02}^{-2}l_y^2\} + (1/2)\hbar S\vec{l}(\partial\vec{l}/\partial t \times \nabla\vec{l}), \quad (2)$$

where $c = 2JSa/\hbar$ is the phase velocity of spin waves and $x_{0j} = a(J/2D_j)^{1/2}$, $j = 1,2$ are characteristic length scales. It is assumed that the anisotropy is high enough to suppress quantum fluctuations, and the ground state is ordered. The magnetization $\vec{m}$ can be expressed via $\vec{l}$ and its derivatives:

$$\vec{m} = (\hbar/4JS)(\vec{l} \times \partial\vec{l}/\partial t) - (1/2)a\nabla\vec{l}. \quad (3)$$

This formula can be obtained either directly by the variation of the full Lagrangian $L\{\vec{m},\vec{l}\}$ in $\vec{m}$ or from (2) by considering an infinitesimal rotation $\delta\vec{\theta}$ in $\vec{l}$ space and using the fact that $\vec{m} \propto \delta\mathcal{L}/\delta\vec{\theta}$ (see Ref. [16] for details).

The model (2) has elementary excitations of two types, kinks and magnons. There are two branches of magnons, with $\vec{l}$ oscillating in the (zx) and (zy) planes, respectively. For both branches the dispersion law has Lorentz-invariant form $\omega_j(k) = (\omega_{0j}^2 + c^2k^2)^{1/2}$, where $\omega_{0j} = c/x_{0j}$ are the activation frequencies, and k is the magnon wave vector.

For analyzing soliton solutions it is convenient to introduce angular variables instead of the unit vector, $l_x + il_y = \sin\theta e^{i\varphi}$, $l_z = \cos\theta$. At $\varphi = \text{const}$ the equations of motion reduce to the sine-Gordon equation for the variable 2θ. Respectively, there are two simplest static soliton solutions, describing π kinks of the vector $\vec{l}$,

$$\cos\theta_0 = \sigma\tanh(x/x_{0j}), \qquad \varphi = \varphi_0, \quad (4)$$

where $\varphi_0 = 0,\pi$ for $j = 1$ and $\varphi_0 = \pm\pi/2$ for $j = 2$; $\sigma = \pm 1$ is the topological charge. Rest energies of the zx and zy kinks are simply related to the corresponding magnon gaps: $E_{0j} = S\hbar\omega_{0j}$. It is worthwhile to remark that in FM's $E_0/\hbar\omega_0 \propto (J/D)^{1/2}$, and kinks are "heavy" particles, in contrast to AFM's, where for realistic S values kinks are rather "light." For $\rho > 0$ the zx kink is energetically disadvantageous and unstable.

For the *purely uniaxial* case ($\rho = 0$) all directions in the (xy) plane are equivalent, and one can construct a dyon solution, where $\vec{l}$ precesses around the z axis with the frequency ω [5,6]:

$$\cos\theta = \sigma\tanh\{(x/x_0)(1 - \omega^2/\omega_0^2)^{1/2}\}, \qquad \varphi = \omega t. \quad (5)$$

Here $x_0 \equiv x_{02}$ and $\omega_0 \equiv \omega_{02}$. Because of the Lorentz invariance, kinks moving with the velocity v can easily be obtained from the $v = 0$ solutions by the substitution $(x,t) \mapsto (\xi,\tau)$, $(\xi,\tau) = (1 - v^2/c^2)^{-1/2}(x - vt, t - vx/c^2)$. The precession frequency ω lies in the interval $-\omega_0 \le \omega \le \omega_0$ and is related to the additional integral of motion, the z component of the total spin $S_z = (\hbar S/a)\int dx\, m_z$, which is simply a conserved momentum canonically conjugate to the φ:

$$S_z/\hbar = \sigma S + S\omega/(\omega_0^2 - \omega^2)^{1/2}. \quad (6)$$

The first term in S_z comes from the $\nabla\vec{l}$ contribution to $\vec{m}$ and is topologically invariant. Semiclassical quantization of the internal motion requires that S_z is quantized in integer steps of $\hbar$, i.e., $S_z = \nu\hbar$ [6,17]. From the properties under time reversal [6] it follows that the quantum number ν must be integer or half integer for integer or half-integer S, respectively. Thus we obtain that $S_z - \sigma S\hbar = n\hbar$, where n is always an integer. For the energy of the dyon solution (5) one can write an expression coinciding with that obtained by Haldane [6]:

$$E_n = \hbar\omega_0(S^2 + n^2)^{1/2}; \quad (7)$$

the energy of a moving dyon with momentum P is $E_n(P) = (E_n^2 + c^2P^2)^{1/2}$. It should be remarked that in the pioneering work of Haldane [6] the contribution to $\vec{m}$ leading to the first term in (6) did not arise, because in that paper Haldane used a different procedure of passing to the continuum limit which did not conserve the total number of degrees of freedom. Thus he arrived at the conclusion that n must be half integer for half-integer S, and that the minimum of energy in that case is reached at $n = 1/2$, i.e., in a state with nonzero precession frequency ω. In our approach n is an integer irrespective of S, and the minimum of energy is always reached at $n = 0$.

Real AFM chains are not purely uniaxial. A small *in-plane anisotropy* is always present, destroying the integral of motion S_z. Let us consider how the transition from dyons (5) to simple sine-Gordon zy kinks (4) takes place when ρ increases. For $\rho \ne 0$ the simplest linear analysis of excited states against a background of a zy kink reveals the existence of a localized magnon mode with the eigenfrequency $\omega_{\text{loc}} = \omega_0\sqrt{\rho}$ and the eigenfunction corresponding to uniform (independent of ξ) oscillations of φ around φ_0. However, in AFM's the range of applicability of the linear approximation is very restricted because of strong quantum fluctuations. The estimation of the amplitude of zero-point fluctuations yields $\langle(\varphi - \varphi_0)^2\rangle \sim 1/S\rho^{1/2}$, so that for realistic values of S fluctuations are not small even at $\rho \sim 1$. The linear approximation is valid only for $\rho S^2 \gg 1$. Zero-point fluctuations drive the oscillator to the nonlinear regime, and therefore localized modes in 1D AFM's should be treated quantum mechanically, with the account taken of nonlinearity. At certain sufficiently small $\rho \sim 1/S^2$, oscillations of φ completely delocalize, transforming into rotations. Note that it is very different from the situation in 1D FM's, where the amplitude of zero-point fluctuations $\langle\Delta\varphi^2\rangle \propto (D/J)^{1/2}$ is rather small and localized modes can be treated classically.

To analyze the transition from the usual kinks to dyons, we note that in both limiting cases $\rho \gg 1$ and $\rho \to 0$ the variable φ does not depend on x; $\varphi = \varphi(t)$. Thus if we are interested in the dynamics of the localized mode only (which is responsible for the transition), we can look for a soliton solution of the form

$$\cos\theta = \sigma \tanh[x/\bar{x}_0(\varphi_s)], \qquad \varphi = \varphi_s(t), \qquad (8)$$

where $\bar{x}_0(\varphi_s) = x_0/(1 + \rho \sin^2\varphi_s)^{1/2}$, and φ_s is treated as a slow variable, provided that the frequency of the localized mode is small compared to ω_0. In our simple Lorentz-invariant model, obtaining moving solutions is trivial, and translational and internal motion are decoupled. The presence of an external magnetic field violates the Lorentz invariance and couples internal and translational degrees of freedom, leading to interesting quantum effects which will be reported elsewhere.

Proceeding to a canonical quantization, we obtain the equation of the wave functions Ψ_n and energy levels E_n of the internal mode,

$$\{-(\hbar^2\omega_0^2/2E_0)\partial^2/\partial\varphi_s^2 + U(\varphi_s)\}\Psi_n = E_n\Psi_n, \qquad (9)$$

where $U(\varphi_s) = E_0(1 + \frac{1}{2}\rho \sin^2\varphi_s)$ is a periodic potential and $E_0 \equiv E_{02}$ is the energy of a static zy kink. This is the well-known Mathieu equation [18], and its solutions depend on the parameter $\rho S^2/4$. At $\rho S^2 \gg 4$ the beginning of the spectrum corresponds to a harmonic oscillator, and higher energy levels transform to those of a free rotator:

$$E_n \simeq \hbar\omega_0 S + \hbar\omega_{\mathrm{loc}}(n + 1/2), \quad E_n \ll \rho E_0/2, \qquad (10a)$$

$$E_n^{(\pm)} \simeq \hbar\omega_0 S + n^2(\hbar\omega_0/2S), \quad E_n \gg \rho E_0/2. \qquad (10b)$$

If $\rho S^2 \ll 4$, which is a more realistic regime for $\rho \ll 1$, then the motion of φ is never constrained, and the energy levels from the very beginning are described by (10b), to the first order in ρ. Recall that (10b) can be obtained from Eq. (7) at $n \ll S$. The range of validity of (9) is the same, $n \ll S$, because the frequency of the localized mode $(E_{n+1} - E_n)/\hbar$ should be small compared to ω_0. Thus at $\rho S^2 \ll 4$ quantum zero-point fluctuations become rotations, and the dynamics is essentially that of a dyon in a purely uniaxial case. One can expect this correspondence to remain the same at a higher excitation level (higher n), so that for $\rho S^2 \ll 4$ the expression (7) will be approximately correct for arbitrary n. For those reasons we expect that dyons can exist even in nonuniaxial AFM's, provided that the magnitude of rhombicity is not too large.

Dyon thermodynamics.—At low temperatures $T \ll E_0$ the statistical mechanics of a dyon gas can be considered phenomenologically, following the approach of Ref. [2]. The distribution function of dyons can be represented in the form

$$w(P,n) = (2\pi\hbar)^{-1} L \exp\{-[E_n(P) + \Sigma_s]/T\}, \qquad (11)$$

where L is the chain length, and Σ_s is the change in the free energy of the magnon gas due to the presence of a kink, which is attributed to the kink self-energy

$$\Sigma_s = (T/2\pi) \sum_{j=1,2} \int dk\, \delta_j'(k) \ln\{1 - e^{-\hbar\omega_j(k)/T}\}. \qquad (12)$$

Here $\delta_j(k)$ is the asymptotic phase shift acquired by a magnon of the jth branch of the continuous spectrum after its interaction with a kink, and the prime indicates differentiation with respect to k. Generally, $\delta_j(k)$ depends also on P and n, but for low temperatures $T \ll E_0$ the main contribution to the thermodynamics comes from dyons with $P \ll E_0/c$ and $n \lesssim S$, and this weak dependence may be neglected. At $n = 0$ the expression for $\delta_j(k)$ is easily found from the exact magnon wave functions against the background of a sine-Gordon kink (4), $\delta_{1,2}(k) \simeq -2 \arctan kx_0$ [2].

The total soliton density $n_s = L^{-1}\sum_n \int dP\, w(P)$ determines the correlation length $\xi_{\mathrm{cor}} = 1/2n_s$ and can be easily calculated for various regimes, depending on the values of $T/\hbar\omega_0$ and ρ. In the *classical linear* case $\rho \gg 4/S^2$ the dyon energy $E_n(P)$ is given by (10a), and for the high-temperature interval $1 \ll T/\hbar\omega_0 \ll S$ we obtain the usual sine-Gordon result [2] $n_s = x_0^{-1}(2E_0/\pi T)^{1/2} e^{-E_0/T}$, often cited in literature without any comments concerning its applicability conditions. In the low-temperature region $T \lesssim \hbar\omega_0$ correction to the kink self-energy Σ_s is exponentially small, so that for n_s we have the expression

$$n_s = S x_0^{-1}(T/2\pi E_0)^{1/2} e^{-E_0/T}, \qquad (13)$$

similar to that obtained by Krumhansl and Schrieffer [1] completely neglecting kink-magnon interaction. This formula naturally appears in the low-temperature limit when magnon degrees of freedom are frozen. It should be pointed out that for AFM's, in contrast to FM's, the temperatures $T < \hbar\omega_0$ are still high enough for the soliton density not to be vanishingly small, because of the relative smallness of the ratio $E_0/\hbar\omega_0$.

In the opposite *nonlinear quantum* regime $\rho \ll 4/S^2$ the dyon energy is approximately described by the expression (7), and at $T \ll \hbar\omega_0 S$ the free rotator formula (10b) can be used. Furthermore, if $T \gg \hbar\omega_0/S$, this rotator can be considered classically. In the high-temperature region $T \gg \hbar\omega_0$ we obtain for the soliton density

$$n_s = (4E_0/Tx_0)e^{-E_0/T}, \qquad (14)$$

which coincides with the exact result for the uniaxial model, obtained by Nakamura and Sasada [19] by the transfer operator technique, thus justifying our phenomenological approach to the statistical mechanics of the dyon gas. In the intermediate temperature range $1/S \ll T/\hbar\omega_0 \ll 1$ we have

$$n_s = (TS^2/E_0 x_0)e^{-E_0/T}, \qquad (15)$$

and for very low temperatures $T \ll \hbar\omega_0/S$ one again obtains the expression (13). We would like to note that formulas (13) and (15) cannot be obtained within the framework of a classical transfer-operator technique, because they, in fact, take into account quantum effects of mode "freezing."

Response functions.—Consider the dyon contribution to the dynamic structure factor (DSF) $S^{\alpha\beta}(Q,\omega)$, which is essentially the Fourier transform of the two-spin correlation function $\langle S^\alpha(z,t)S^\beta(z',0)\rangle$. Usual sine-Gordon kinks are known to lead to the central peak (CP) in the DSF, around $\omega = 0$ [3]. In the case of AFM's, the main contribution to the DSF comes from the correlator of the antiferromagnetism vector $\vec{l}$ and is concentrated around the magnetic Bragg wave vector $Q_B = \pi/a$ (the contribution of $\vec{m}$ is concentrated near $Q = 0$ and is D/J times smaller in intensity).

The longitudinal (with respect to the easy axis) component S^{zz} remains almost unaffected by the internal kink dynamics, and we will be interested only in transverse components. If $\rho S^2 \gg 4$, the localized mode is "hard" and contributes only to the high-frequency region, so one can neglect it when describing the CP. Then $S^{xx} \simeq 0$, and for S^{yy} we obtain the usual Gaussian-shaped CP [3], $S^{yy}(Q_B + q, \omega) \simeq f_G(q, \omega)$, where

$$f_G(q, \omega) \simeq \frac{(2\pi)^{1/2} L n_s}{q v_T} |F_\perp(q)|^2 \exp\left\{-\frac{\omega^2}{2q^2 v_T^2}\right\}.$$

The half-width of such a CP is $\Gamma \simeq q v_T$. Here $v_T = c(T/E_0)^{1/2}$ is the rms velocity of a kink, and $F_\perp(q) = \pi \cosh^{-1}(\pi q x_0/2)$ is the transverse form factor describing the kink shape.

In the "quantum" case $\rho S^2 \ll 4$ the system is almost axially symmetrical, and $S^{xx} \simeq S^{yy} = S^\perp$. The resulting expression for $S^\perp$ can be written in the form

$$S^\perp(Q_B + q, \omega) \simeq (2Z_d)^{-1} \sum_{n=0}^{\infty} e^{-E_n/T} \{f_G(q, \omega - \Omega_n) + e^{-\hbar\Omega_n/T} f_G(q, \omega + \Omega_n)\}, \quad (16)$$

where $E_n = \hbar\omega_0(S^2 + n^2)^{1/2}$ are the dyon energy levels, and $Z_d = \sum_n e^{-E_n/T}$ is the partition function. This formula describes a set of Gaussian peaks centered at the transition frequencies $\Omega_n = (E_{n+1} - E_n)/\hbar$, with the dispersion $q v_T$ each. The envelope function of these peaks is a CP with approximately Gaussian form and dispersion $\Gamma \simeq \omega_T$, where $\omega_T = \omega_0(T/E_0)^{1/2}$ has the meaning of an average thermal precession frequency. The expression (16) is asymmetric in ω, and at extremely low temperatures $T \lesssim \hbar\omega_0/S$ only the peak at $\omega = \Omega_0$ survives.

For quasi-1D AFM compound $CsMnI_3$, according to Ref. [11], $S = 5/2$, $J \simeq 198$ GHz, $D_1 \simeq D_2 \simeq 1.07$ GHz, and the estimation gives $\Omega_0 \simeq 28$ GHz. This value lies in the frequency range which is accessible rather to the ESR methods (note that transitions between rotator levels can occur without momentum transfer, i.e., at $Q = 0$, so that ESR can be used for their detection). Neutron experiments have low resolution and will probably be able to detect only the envelope CP with the half-width $\Gamma = \omega_T$ independent of the scattering vector q, in contrast to the usual soliton CP with $\Gamma = q v_T$.

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