Nonlinear Excitations on a Quantum Ferromagnetic Chain

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We use a spin-coherent representation to derive the spectrum of nonlinear excitations in a spin-S quantum ferromagnetic Heisenberg chain in the continuum limit. Quantum effects split the semiclassical spectrum into two branches—a lower branch of spin-wave-like, large-width solitary waves with negligible quantum corrections for all S, and an upper branch of particlelike, small-width solitary waves subject to significant quantum corrections for low S. The stability of these excitations is briefly discussed.

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The spin-S, classical, isotropic, ferromagnetic Heisenberg chain[1] in the continuum limit is a completely integrable nonlinear system whose spin-evolution equation has exact soliton solutions. These are the natural nonlinear excitations of the system. Bethe[2] obtained the exact multimagnon bound-state spectrum of the quantum, discrete, spin-$\frac{1}{2}$ chain, using an *Ansatz* for the form of the spin eigenstates. Semiclassical quantization (e.g., via path integration)[3] of a classical soliton yields an energy spectrum (for general S) formally identical to the continuum limit of the Bethe-*Ansatz* spectrum. This suggests that the semiclassically quantized solitons of the classical field theory correspond to the bound states of the quantum problem. This correspondence extends to other quantum systems such as the sine-Gordon and nonlinear Schrödinger field theories.[4] However, it is not always physically illuminating to calculate quantum corrections in a path-integral approach, and the validity of the semiclassical approximation is often questioned,[5] especially for small S values. In this Letter we present an alternative formalism for treating quantum spin dynamics which also clarifies quantitatively the role of the quantum effects on soliton motion.

We study soliton dynamics in the isotropic, quantum Hamiltonian $\hat{H} = -J\sum_n \hat{\mathbf{S}}_n \cdot \hat{\mathbf{S}}_{n+1}$ by analyzing the spin-operator evolution equation in Radcliffe's spin-coherent representation.[6] Earlier coherent-state treatments[7–9] use a severely truncated Holstein-Primakoff expansion for $\hat{\mathbf{S}}_n^{\pm}$ and further approximate $\hat{H}$ by a Hamiltonian which is biquadratic in *boson* operators. Working in Glauber's coherent state representation and making a small-amplitude approximation, one then finds solitary-wave profiles identical to classical solitons. The total energy and magnetization are found approximately. However, the total momentum (which is also a constant of the motion) has not been considered in this approach, probably because the boson representation does not provide a natural basis for its construction. Moreover, it is evident that the truncation of the operator expansion and the subsequent approximations distort the nonlinearity of the system. In contrast, we work here directly with the spin operators, make no approximations to $\hat{H}$, develop and use an exact nonlinear equation for the quantum system, construct the momentum operator $\hat{P}$, and finally, also obtain the energy-momentum relation for the solitons. The spin-coherent representation thus appears to be the one best suited for the analysis of quantum effects on the nonlinear excitations of spin systems—the method is readily applied to spin symmetries other than that treated here.

Details of our work will be published elsewhere, but the principal resuls are as follows: (1) The solutions of the exact nonlinear equation in the spin-coherent representation are identical in form to classical solitons, without any small-amplitude approximation. (2) The Bethe-*Ansatz*-like semiclassical soliton spectrum obtains in the small-amplitude regime for all S. (3) Quantum corrections to the spectrum[5] are negligible for large-width, small-amplitude spin-wave-like excitations for all S. They are significant for small-width, large-amplitude, particlelike excitations for small S. For general S, the spectrum thus has *two* branches (representing these two types of excitations), with a crossover at a certain "critical" width (and energy). (4) The quantum solitary wave is unstable as a means of energy transport when its width lies within a range of values around the critical width, and stable otherwise. This instability range decreases as S increases.

We work with the direct product states $|\mu\rangle = \otimes_n |\mu_n\rangle$ where the spin-coherent state $|\mu_n\rangle = (1 + |\mu_n|^2)^{-S}\exp(\mu_n \hat{S}_n^-)|0\rangle$, $\mu_n \in C$, and $|0\rangle$ is defined by $\hat{S}_n^z|0\rangle = S|0\rangle$. The states $|\mu_n\rangle$ are normalized, nonorthogonal, and overcomplete. The diagonal matrix element $\langle\mu|\hat{A}|\mu\rangle$ of an operator $\hat{A}$ is denoted by $\langle\hat{A}\rangle$. These elements are known to be good operator representatives.[10] It is convenient to use the parametrization[6] $\mu_n = \tan(\frac{1}{2}\theta_n)\exp(i\phi_n)$, so that

$$\langle \hat{S}_n^x \rangle = S\sin\theta_n\cos\phi_n, \quad \langle \hat{S}_n^y \rangle = S\sin\theta_n\sin\phi_n, \quad \langle \hat{S}_n^z \rangle = S\cos\theta_n,$$

while

$$\langle (\hat{S}_n^z)^2 \rangle = S(S-\tfrac{1}{2})\cos^2\theta_n + \tfrac{1}{2}S.$$

The equation of motion is

$$i\partial_t \hat{S}_n^+ = J\hbar^{-1}[(\hat{S}_{n-1}^z + \hat{S}_{n+1}^z)\hat{S}_n^+ - \hat{S}_n^z(\hat{S}_{n-1}^+ + \hat{S}_{n+1}^+)], \tag{1}$$

which yields a nonlinear c-number equation for the diagonal matrix elements *with the same physical content.* In the continuum limit, we obtain, after some algebra, the coupled equations

$$(\sin\theta)\partial_t\phi = J\hbar^{-1}a^2[\partial_{xx}\theta - \sin\theta\cos\theta(\partial_x\phi)^2], \quad \partial_t\theta = -J\hbar^{-1}a^2[\sin\theta(\partial_{xx}\phi) + 2\cos\theta(\partial_x\theta)(\partial_x\phi)], \tag{2}$$

where a denotes the lattice spacing. In terms of the canonical variables[1] $p = \cos\theta$ and $q = \phi$, Eqs. (2) are identical to the evolution equations for the *classical* continuum chain (after a redefinition of the constants). For the boundary conditions $\cos\theta \to 1$ as $|x| \to \infty$, Eqs. (2) have the single-soliton solution given by[1]

$$\sin^2(\tfrac{1}{2}\theta) = (1-\alpha^2)\,\mathrm{sech}^2[(x - vt - x_0)/\Gamma]$$

and

$$\phi = \phi_0 + \omega t + \hbar v(x - vt)/(2JSa^2) + \tan^{-1}\{(2JSa^2/\hbar v\Gamma)\tanh[(x - vt - x_0)/\Gamma]\}, \tag{3}$$

where x_0 and ϕ_0 are constants. The translational velocity of the soliton is v, its intrinsic rotational frequency is ω, its amplitude is $(1-\alpha^2)$, and its width is $(JSa^2/\hbar\omega)^{1/2}(1-\alpha^2)^{-1/2} = \Gamma$, where $\alpha = v/(4J\hbar^{-1}a^2S\omega)^{1/2}$, $0 \leq \alpha \leq 1$. We also find

$$\langle \hat{S}^z(x,t) \rangle = S\{1 - 2(1-\alpha^2)\,\mathrm{sech}^2[(x - vt - x_0)/\Gamma]\}. \tag{4}$$

The total energy and magnetization corresponding to solution (3) are

$$E = \langle \hat{H} \rangle = 4(JS^3\hbar\omega)^{1/2}(1-\alpha^2)^{1/2} \tag{5}$$

and

$$M = \langle \hbar \textstyle\sum_n (\hat{S}_n^z - S) \rangle = -4(JS^3\hbar/\omega)^{1/2}(1-\alpha^2)^{1/2}. \tag{6}$$

Hence

$$E = 16JS^3\hbar(1-\alpha^2)/|M| = \omega|M|. \tag{7}$$

Defining the classical constants according to $J\hbar^2 \to J_{\mathrm{cl}}$, $S\hbar \to S_{\mathrm{cl}}$ and then passing to the continuum limit, we find that (5) and (6) are formally identical to the classical expressions. This happens essentially because E and M (unlike the momentum P, to be defined below) involve operators that are *linear* in the spins at any single site.

Our strategy has been to work with the spin-coherent respresentation for the discrete chain, take the diagonal matrix elements of operators, and then pass to the continuum limit. Thus, in order to find the energy-momentum relation, we must first construct the momentum operator $\hat{P}$ in the discrete case. For the classical, continuous chain, the momentum—the infinitesimal generator of translations—is given by[1,3]

$$P_{\mathrm{cl}} = a^{-1}\int dx\,(S_{\mathrm{cl}}^x \overleftrightarrow{\partial}_x S_{\mathrm{cl}}^y)/(S_{\mathrm{cl}} + S_{\mathrm{cl}}^z), \tag{8}$$

where $\mathbf{S}_{\mathrm{cl}}$ has the dimensions of angular momentum. To construct the correct quantum analog, we discretize (8), replace $(S_{\mathrm{cl}}^i)_n$ by $\hbar\hat{S}_n^i$ $(i = x,y,z)$ and S_{cl} by $\hbar\langle\hat{\mathbf{S}}^2\rangle^{1/2} = \hbar[S(S+1)]^{1/2}$, and finally symmetrize the resulting expression to ensure that $\hat{P}$ is Hermitian. ($\hat{\mathbf{S}}_n$ is dimensionless). Thus

$$\hat{P} = (\hbar/2a)\textstyle\sum_n\{(\hat{S}_n^x\hat{S}_{n+1}^y - \hat{S}_{n+1}^x\hat{S}_n^y)/[S^{1/2}(S+1)^{1/2} + \hat{S}_n^z] + \mathrm{H.c.}\}. \tag{9}$$

To find $P = \langle \hat{P} \rangle$, we must expand the inverse operator in (9) in powers of $\hat{S}_n^z$. If, in this expansion, we make the approximation

$$(\hat{S}_n^z)^r \simeq \langle (\hat{S}_n^z)^r \rangle \simeq \langle \hat{S}_n^z \rangle^r \quad (r = 1, 2, \ldots)$$

for all S, we obtain

$$P = (4S\hbar/a)\sin^{-1}(1-\alpha^2)^{1/2}. \tag{10}$$

Combining Eqs. (7) and (10) yields the dispersion relation

$$E=(16JS^3\hbar/|M|)\sin^2(Pa/4S\hbar)\rightarrow(16J_{\rm cl}S_{\rm cl}^3/|M|)\sin^2(Pa/4S_{\rm cl}), \tag{11}$$

where $|P|\leqslant 2\pi S_{\rm cl}/a$. Expression (11) is again just the classical result,[1] obtained because the above mean-field-like approximation amounts to neglect of quantum fluctuations—a procedure justified only in the small-amplitude limit. Moreover, we find that the group velocity is

$$c_g(P,M)\equiv(\partial E/\partial P)_M=v, \tag{12}$$

the soliton velocity itself, for all S.

On the other hand, we can in principle calculate $\langle\hat{P}\rangle$ *exactly* for any S. (The calculation becomes increasingly tedious as S increases.) For low values of S, we find, for $S=\frac{1}{2}$,

$$Pa=2\sqrt{3}\hbar\alpha(1-\alpha^2)^{1/2}; \tag{13a}$$

for $S=1$,

$$Pa=2\hbar\alpha(1-\alpha^2)(4.90-2.66\alpha^2); \tag{13b}$$

for $S=\frac{3}{2}$,

$$Pa=9\hbar\alpha(1-\alpha^2)^{1/2}[0.83+0.32(1-\alpha^2)+0.68(1-\alpha^2)^2+0.88(1-\alpha^2)^3]. \tag{13c}$$

Figure 1 shows how $Pa/2\pi S\hbar$ varies with α. For each S there is a *single* maximum in P which shifts as S increases towards the limiting value $2\pi S_{\rm cl}/a$ of the classical curve. For each value of P, there are *two* values of α (in contrast to the classical case), and this implies two possible soliton widths Γ. Figure 2 shows the E-P dispersion relations for $S=\frac{1}{2}$ and $S=\frac{3}{2}$, obtained (with $M=$const) by eliminating α between Eqs. (7) and (13). (The curve for $S=1$ lies in between these curves.) Different scales have been chosen for the two cases so that the corresponding semiclassical spectra are identical (for ease of comparison). The quantum spectrum consists of two branches, with a crossover at a critical energy $E_c(S)$. Since $E=4JS^2a/\Gamma$, we see that quantum effects dominate for the small-Γ, particlelike excitations of the upper branch, and are relatively unimportant[5] for the large-Γ, magnonlike modes of the lower branch. The latter expands with increasing S, until it takes over completely in the classical limit ($S\rightarrow\infty,\hbar\rightarrow 0$). The group velocity c_g has opposite signs for the two branches with $|c_g|\rightarrow\infty$, as $E\rightarrow E_c(S)$. This might appear to be unphysical, but a heuristic argument[11] shows that for $|c_g|\geqslant v_{\rm max}=(4J\hbar^{-1}S\omega a^2)^{1/2}$, the excitations become unstable—essentially because energy transport cannot be physically associated with solitons in this regime. For $S=\frac{1}{2}$, this implies instability for $Pa/\hbar\gtrsim 0.7$. If this argument is taken seriously, there is an intermediate range of energies (and widths) for which the solitons are unstable; for low spin values, stable quantum solitons exist only for small P. As S increases, the range of instability narrows. Quantum fluctuations thus strongly affect the stability of the solitons: Ignoring such effects (the semiclassical approximation) yielded $c_g=v$ [Eq. (12)], suggesting stable solitary waves for

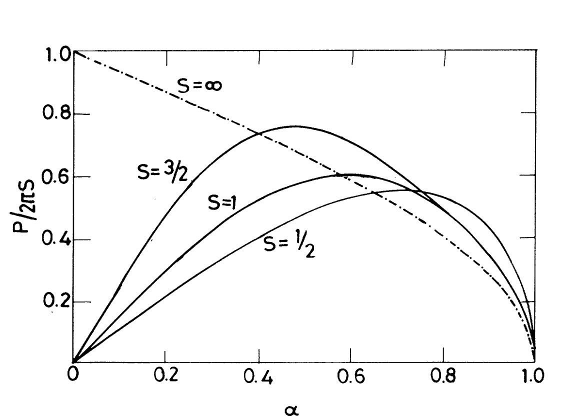

FIG. 1. The (scaled) momentum $P/(2\pi S)$ (units of $\hbar a^{-1}$) vs α.

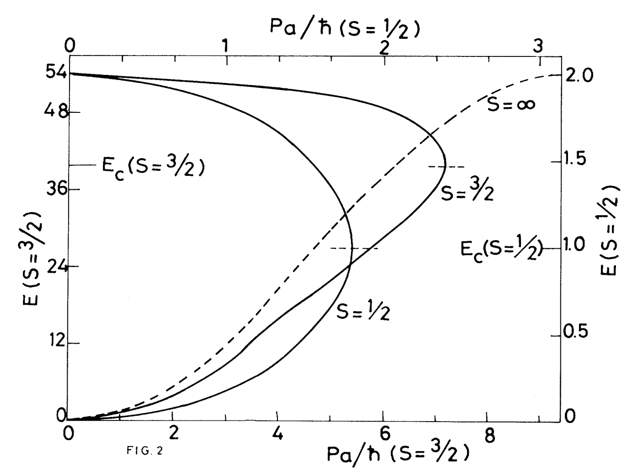

FIG. 2. Soliton energy E (units of $J\hbar|M|^{-1}$) vs momentum P (units of $\hbar a^{-1}$).

all P. (Their stability can be established independently in this case.) A rigorous stability analysis of the quantum case presents a complicated numerical problem which we have not yet solved.

In the presence of an external magnetic field in the z direction, the parameter ω in the soliton solution becomes $\omega+\omega_0$ where ω_0 is proportional to the field. It would be interesting to investigate experimentally the existence and stability of the nonlinear excitations predicted here, using ω_0 as a control parameter for the soliton width, amplitude, and energy.

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