Nonlinear dynamics of a quantum ferromagnetic chain: Spin-coherent-state approach

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The spin evolution equation of an isotropic, quantum ferromagnetic Heisenberg chain is analyzed in the continuum approximation using spin-coherent states. The advantages of this approach are discussed. Magnetic solitary-wave solutions are found, and the expectation values of the energy, momentum, and angular momentum corresponding to these solutions are determined. The energy-momentum dispersion relation for the nonlinear excitations is derived. The semiclassical spectrum is shown to arise when quantum effects are neglected by using a random-phase approximation to calculate certain expectation values. On including the quantum effects, it is found that the spectrum comprises two branches: a lower-energy branch of spin-wave-like, small-amplitude solitary waves with small quantum corrections, and a higher branch of particlelike large-amplitude solitary waves subject to significant quantum corrections for small S values. A heuristic discussion of the stability of these excitations is presented. A physical interpretation of the dispersion relation obtained is given.

I. INTRODUCTION

An analysis of the dynamical properties of a Heisenberg ferromagnetic chain is a nonlinear problem of considerable interest both experimentally and theoretically, in the context of one-dimensional magnetic materials.[1] For the spin-S *classical* Heisenberg chain, complete integrability and the existence of soliton solutions have been established in the continuum model, using the inverse-scattering method.[2] The exact energy-momentum dispersion relation for these solitons (which may be regarded as the natural nonlinear excitations of the classical system) is also known.[3] In contrast, treatments[4–6] of the soliton dynamics in the *quantum* Heisenberg chain have involved various truncating approximations in the evolution equation for the spin operators. These truncations distort the true nonlinearity of the system, and are usually uncontrollable approximations. Furthermore, these earlier approaches to the dynamics have not dealt with the dispersion relation for the nonlinear excitations in the quantum (continuum) model, for reasons to be explained below. There is thus a clear need for an analysis of the quantum-mechanical problem that does not share these drawbacks, and which also yields the energy-momentum relationship satisfied by the solitons propagating in the system.

The purpose of this work is to show that localized nonlinear excitations (i.e., magnetic solitary waves) propagate in the continuum approximation of the quantum spin chain, to derive their dispersion relation and finally to compare these results with those for the classical model. A summary of our principal results has been published in Ref. 7.

The paper is organized as follows: We use Radcliffe's spin-coherent representation[8,9] (SCR) to analyze the spin operator evolution equation for the isotropic, quantum ferromagnetic Heisenberg Hamiltonian

$$\hat{H} = -J\sum_n \hat{\mathbf{S}}_n \cdot \hat{\mathbf{S}}_{n+1} \ .$$

The advantages of this approach for the problem under consideration are described in Sec. II. In Sec. III, the diagonal matrix element in the SCR of the quantal spin evolution equation is shown to yield a nonlinear c-number equation, which is exact in the sense that it displays the full nonlinearity in the system. In the continuum approximation, this equation supports solitary wave solutions, which are displayed. In Sec. IV, these solutions are used to determine the corresponding expectation values of the constants of motion—the energy E, the momentum P, and the angular momentum M. (Some relevant intermediate steps in the calculation are given in the Appendices.) The dispersion relation for the excitations is presented in Sec. V. In Sec. VI, the results obtained are physically interpreted and compared with those found in the semiclassical approximation.

II. SPIN-COHERENT REPRESENTATION

Earlier calculations[4–6] on the soliton dynamics of quantum spin Hamiltonians begin with the Holstein-Primakoff (boson-operator) expansion[10] for the raising operator $\hat{S}_n^+$ truncated as follows:

$$\hat{S}_n^+ = (2S)^{1/2}(1 - a_n^\dagger a_n/2S)^{1/2} a_n \simeq (2S)^{1/2}(1 - a_n^\dagger a_n/4S) a_n \ . \tag{2.1}$$

The Hamiltonian concerned is further approximated by one which is biquadratic in the boson operators. (We note that these approximations are at best physically justifiable only at sufficiently low temperatures, when $\langle a_n^\dagger a_n \rangle /2S$ is expected to be much smaller than unity.) The diagonal matrix element of this equation between (boson) coherent states[11] defined by the direct product $|z\rangle = \otimes_{n=1}^N |z_n\rangle$, where $a_n|z_n\rangle = z_n|z_n\rangle$ yields a c-number evolution equation for the eigenvalue z_n. In the continuum approximation $z_n(t) \to z(x,t)$, this leads to either the usual nonlinear Schrödinger equation with a cubic nonlinearity, or a modified one[5] with a different nonlinearity, depending on the type of truncation used. Typically, solitary-wave solutions can be shown to exist in the small-amplitude approximation. The corresponding expectation values of the total energy and angular momentum turn out to be identical to the classical expressions. However, the boson-operator formalism does not provide a natural framework for calculating the expectation value of the total momentum, the third constant of the motion for the spin chain. This is why it has not been possible in this approach to obtain any information on the energy-momentum dispersion relation for the excitations. It is also evident that the truncation of the operator expansion, and the subsequent approximations, severely distort the nonlinearity of the problem once one goes beyond the small amplitude limit.

Analogous to the usual boson coherent state[11] $|z_n\rangle$, it is possible to define[8] a spin-coherent state $|\mu_n\rangle$ at each site n, according to

$$|\mu_n\rangle = (1+|\mu_n|^2)^{-S}\exp(\mu_n \hat{S}_n^-)|0\rangle_n \ , \qquad (2.2)$$

where $\hat{S}_n^-$ is the spin lowering operator, $\hat{S}_n^z|0\rangle_n = S|0\rangle_n$, and the eigenvalue $\mu_n \in C$. The spin-coherent states of the system of N spins are direct product states

$$|\mu\rangle = \bigotimes_{n=1}^{N} |\mu_n\rangle \ . \qquad (2.3)$$

The states $|\mu_n\rangle$ are normalized, but nonorthogonal and overcomplete. We have

$$\langle \lambda_n|\mu_n\rangle = (1+\lambda_n^*\mu_n)^{2S}/(1+|\lambda_n|^2)^S(1+|\mu_n|^2)^S \ , \qquad (2.4)$$

$$\pi^{-1}(2S+1)\int d^2\mu_n (1+|\mu_n|^2)^{-2}|\mu_n\rangle\langle\mu_n| = 1 \ . \qquad (2.5)$$

In the calculations to follow, it turns out to be more convenient[8] to use the parametrization

$$\mu_n = \tan(\theta_n/2)\exp(i\phi_n) \ ,$$

where

$$0 \le \theta_n \le \pi$$

and

$$0 \le \phi_n < 2\pi \ .$$

Then

$$|\mu_n\rangle \to |\theta_n,\phi_n\rangle = (\cos\tfrac{1}{2}\theta_n)^{2S} \times \exp[\tan(\tfrac{1}{2}\theta_n)\exp(i\phi_n)\hat{S}_n^-]|0\rangle_n \ , \qquad (2.6)$$

and Eq. (2.5) becomes

$$(4\pi)^{-1}(2S+1)\int d\theta_n \int d\phi_n \sin\theta_n |\theta_n,\phi_n\rangle\langle\theta_n,\phi_n| = 1 \ . \qquad (2.7)$$

The diagonal matrix elements of the single-site spin operators are given by

$$\langle\theta_n,\phi_n|\hat{S}_n^+|\theta_n,\phi_n\rangle = S\sin\theta_n\exp(i\phi_n) \ ,$$
$$\langle\theta_n,\phi_n|\hat{S}_n^z|\theta_n,\phi_n\rangle = S\cos\theta_n \ . \qquad (2.8)$$

These expectation values are formally identical to the classical values. However, this is no longer true for higher powers of products of single-site operators—for example,

$$\langle(\hat{S}_n^z)^2\rangle = S(S-\tfrac{1}{2})\cos^2\theta_n + \tfrac{1}{2}S \ , \qquad (2.9)$$

in contrast to the classical values $(S\cos\theta_n)^2$.

The SCR is well suited for the study of spin dynamics in many respects. First and foremost, there is no need to truncate the given Hamiltonian as in a boson-operator transformation, so that the exact nonlinear spin evolution may be dealt with. Second, the construction of the momentum operator and the calculation of its expectation value are feasible in this approach, leading to the determination of the soliton dispersion relation. Finally, a comparison of this relation with its classical counterpart helps clarify the extent and nature of quantum effects in the behavior of the solitons.

For large-N magnetic systems, using the representation (2.3) would be well justified even for small S. We note that the SCR has been used recently by Mead and Papanicolaou[12] to find the *spin-wave* excitation spectrum of a spin-one easy-plane ferromagnet ($CsNiF_3$) using a certain Gaussian approximation for the diagonal matrix elements of the Hamiltonian. Their results agree with those found using the Holstein-Primakoff transformation. They further establish that quantum corrections to the spin-wave dispersion relation are small. Our results for the *soliton* modes in a quantum isotropic ferromagnet will suggest that these corrections are again small for low-amplitude (large-width) spin-wave-like solitons, becoming negligible for large values of S. However, quantum corrections will be found to be significant for particlelike amplitude solitons, especially for small S.

III. SOLITON SOLUTIONS

The isotropic ferromagnetic Hamiltonian we consider is

$$\hat{H} = -J\sum_n \hat{\mathbf{S}}_n\cdot\hat{\mathbf{S}}_{n+1} \ . \qquad (3.1)$$

The equation of motion for the raising operator is

$$i\partial_t\hat{S}_n^+ = J\hbar^{-1}[(\hat{S}_{n-1}^z+\hat{S}_{n+1}^z)\hat{S}_n^+ - \hat{S}_n^z(\hat{S}_{n-1}^+ + \hat{S}_{n+1}^+)] \ . \qquad (3.2)$$

The importance of an overcomplete set of states as a tool in the study of quantum dynamics has been discussed in a more general framework by Klauder.[13] The *diagonal* matrix elements of operators in a coherent-state representation can be regarded as good operator representatives.[11] Using this property, the physical content of the operator equation (3.2) can be transferred to the coupled c-number equations for the real variables θ_n and ϕ_n by taking the diagonal matrix element of Eq. (3.2) in the spin-coherent state

$$|\Omega\rangle = \bigotimes_{n=1}^{N} |\theta_n,\phi_n\rangle .$$

We get, with the help of Eqs. (2.8),

$$\sin\theta_n \partial_t \phi_n = J\hbar^{-1} S\{\cos\theta_n[\sin\theta_{n+1}\cos(\phi_{n+1}-\phi_n) + \sin\theta_{n-1}\cos(\phi_{n-1}-\phi_n)] - \sin\theta_n(\cos\theta_{n+1}+\cos\theta_{n-1})\} \quad (3.3a)$$

and

$$\partial_t \theta_n = J\hbar^{-1} S[\sin\theta_{n+1}\sin(\phi_n-\phi_{n-1}) + \sin\theta_{n-1}\sin(\phi_n-\phi_{n-1})] . \quad (3.3b)$$

In the continuum approximation—which is valid if the solutions θ and ϕ do not vary appreciably within the nearest-neighbor distance a on the chain—Eqs. (3.3) become

$$(\sin\theta)\partial_t\phi = J\hbar^{-1}a^2[\partial_{xx}\theta - \sin\theta\cos\theta(\partial_x\phi)^2] , \quad (3.4a)$$

and

$$\partial_t\theta = -J\hbar^{-1}a^2[(\sin\theta)\partial_{xx}\phi + 2\cos\theta(\partial_x\theta)(\partial_x\phi)] . \quad (3.4b)$$

Equations (3.4) are identical in form to those in the continuum model for the isotropic classical chain[3] (after a redefinition of the constants). To solve the equations, it turns out to be convenient to reexpress them in terms of the canonical variables p and ϕ, where $p=\cos\theta$. For the boundary conditions $\cos\theta \to 1$, as $|x| \to \infty$, Eqs. (3.4) have the solitary wave solution[3] given by

$$\sin^2(\tfrac{1}{2}\theta) = (1-\alpha^2)\text{sech}^2[(x-vt-x_0)/\Gamma] , \quad (3.5a)$$

and

$$\phi = \phi_0 + \omega t + (2JSa^2)^{-1}\hbar v(x-vt) + \tan^{-1}\{(2JSa^2/\hbar v\Gamma)\tanh[(x-vt-x_0)/\Gamma]\} , \quad (3.5b)$$

where x_0 and ϕ_0 are constants. The solitary wave has a translational velocity v, intrinsic rotational frequency ω and amplitude $(1-\alpha^2)$. Its width Γ is given by

$$\Gamma = (JSa^2/\hbar\omega)^{1/2}(1-\alpha^2)^{-1/2} , \quad (3.6)$$

where

$$\alpha = v/(4J\hbar^{-1}a^2 S\omega)^{1/2}, \quad 0 \le \alpha \le 1 . \quad (3.7)$$

From Eqs. (2.8) and (3.5a), we have

$$\langle \hat{S}^z(x,t)\rangle = S\{1-2(1-\alpha^2)\text{sech}^2[(x-vt-x_0)/\Gamma]\} . \quad (3.8)$$

We also have

$$(\partial_x\phi) = \hbar v/[JSa^2(1+\cos\theta)] , \quad (3.9)$$

a result that will be used subsequently.

One may ask at this stage whether the solitary wave described by Eqs. (3.5) represents a "strict" soliton.[14] It is well known that the classical spin evolution equation $\partial_t \mathbf{S} = \mathbf{S}\times\mathbf{S}_{xx}$ can be proved to be (gauge) equivalent[15] to the cubic nonlinear Schrödinger equation, which has strict soliton solutions.[16] We have seen that, on using states $|\theta_n,\phi_n\rangle$ defined in Eq. (2.6), the quantum spin evolution equation (3.2) leads in the continuum approximation, to the *coupled* equations for θ, ϕ in Eq. (3.4), which can be solved exactly to give solitary-wave solutions. If instead, we work with states $|\mu_n\rangle$ defined in Eq. (2.2) and use the continuum approximation, we obtain a *single* nonlinear Schrödinger-type equation for the complex quantity $\mu(x,t)$, which has complicated nonlinear terms. Finding a solitary-wave solution for this equation without making a small-amplitude approximation is not an easy task, which is why the parametrization in terms of θ and ϕ was preferred. Having found the exact solutions for θ and ϕ, the corresponding solutions for $\mu(x,t)$ is readily derived from Eqs. (3.5):

$$\mu(x,t) = \tan[\tfrac{1}{2}\theta(x,t)]\exp[i\phi(x,t)] = (1-\alpha^2)^{1/2}\{\alpha^2+\sinh^2[(x-vt-x_0)/\Gamma]\}^{-1} \times \exp[i\phi(x,t)] , \quad (3.10)$$

where $\phi(x,t)$ is given by Eq. (3.5b). This is a pulse-type solitary-wave profile for $\mu(x,t)$. Since the equation for $\mu(x,t)$ does not appear to be readily reducible to a Lax-pair form,[14] it is difficult to decide whether the solitary wave of Eq. (3.10) is indeed a soliton in the strict sense. We have used the term merely in the sense of a localized nonlinear excitation in the present work.

The solution for $\mu(x,t)$ may be compared with that for $z(x,t)$ obtained in earlier work using a truncated Holstein-Primakoff expansion and the conventional boson-coherent states. The two agree only in the small-amplitude (θ) regime, as is expected.

IV. TOTAL ENERGY, ANGULAR MOMENTUM AND MOMENTUM

With the one-soliton solution of Eqs. (3.5) at hand, we can directly calculate two of the constants of motion—the expectation values E and M of the total energy and angular momentum. Using Eqs. (2.8), we have

$$E = \langle\hat{H}\rangle = -JS^2\sum_n[\sin\theta_n\sin\theta_{n+1}\cos(\phi_{n+1}-\phi_n) + \cos\theta_n\cos\theta_{n+1}] . \quad (4.1)$$

In the continuum approximation we have

$$E = \tfrac{1}{2}JSa^2\int_{-\infty}^{+\infty}[(\partial_x\theta)^2 + \sin^2\theta(\partial_x\phi)^2]dx . \quad (4.2)$$

With the help of Eqs . (3.5)–(3.9) we then find

$$E = 4(JS^3\hbar\omega)^{1/2}(1-\alpha^2)^{1/2} , \quad (4.3)$$

where the parameter α has been defined in Eq. (3.7). Similarly, we find

$$M=\left\langle \hbar\sum_n (\hat{S}^z_n - S)\right\rangle \to -\hbar S\int_{-\infty}^{+\infty}\sin^2(\theta/2)d\theta \ , \qquad (4.4)$$

which gives

$$M=-4(JS^3\hbar/\omega)^{1/2}(1-\alpha^2)^{1/2}$$
$$=-4\hbar(JS^3/\hbar\omega)^{1/2}(1-\alpha^2)^{1/2} \ . \qquad (4.5)$$

Therefore

$$E=\omega|M| \ . \qquad (4.6)$$

For the purpose of determining the dispersion relation (to be derived below), it is convenient to write

$$E=16JS^3\hbar(1-\alpha^2)/|M| \ . \qquad (4.7)$$

Recalling Eq. (3.6) for the soliton width Γ, we may also write

$$E=4JS^2a/\Gamma \ . \qquad (4.8)$$

Defining classical parameters according to

$$J\hbar^{-2}=J_{\rm cl}, \quad S\hbar=S_{\rm cl} \ , \qquad (4.9)$$

we note that the expressions found above for E and M are formally identical to the corresponding classical expressions.[3] This happens essentially because E and M involve operators that are of first order in the spins at any given site—recall the comment following Eq. (2.8). This feature does not carry over to the case of the total momentum P, as we shall see.

Our procedure has been to begin with the operators pertaining to a discrete chain, calculate their diagonal matrix elements in the SCR and then use the continuum approximation. To be consistent, we must therefore construct the total momentum operator $\hat{P}$ for a *discrete* chain. There appears to be no simple expression[17] in the literature for this object, for general S. We have chosen to define $\hat{P}$ by the following procedure: For the *classical, continuous* chain, $\hat{P}$, the infinitesimal generator of translations, is given by[18]

$$P_{\rm cl}=a^{-1}\int dx(S^x_{\rm cl}\overleftrightarrow{\partial}_x S^y_{\rm cl})/(S_{\rm cl}+S^z_{\rm cl}) \ , \qquad (4.10)$$

where $S_{\rm cl}$ has the dimensions of angular momentum [see Eq. (4.9)]. This expression is first discretized, and the quantum analog of the result is constructed by the replacements

$$(S^i_{\rm cl})_n \to \hbar\hat{S}^i_n \quad (i=x,y,x) \ ,$$

and

$$S_{\rm cl}\to\hbar\langle\hat{\mathbf{S}}^2\rangle^{1/2}=\hbar[S(S+1)]^{1/2} \ , \qquad (4.11)$$

using the correspondence principle. Finally, the operator obtained in this way is symmetrized to remove any ambiguities in the order of operators. This simultaneously ensures that $\hat{P}$ is Hermitian. (Note that $\hat{\mathbf{S}}_n$ is dimensionless.) We get

$$\hat{P}=(\hbar/2a)\sum_n\{(\hat{S}^x_n\hat{S}^y_{n+1}-\hat{S}^x_{n+1}\hat{S}^y_n)$$
$$\times[S^{1/2}(S+1)^{1/2}+\hat{S}^z_n]^{-1}+\text{H.c.}\} \ . \qquad (4.12)$$

This expression for $\hat{P}$, although approximate, has been constructed using a logical procedure, and is therefore expected to yield physically relevant results in the continuum approximation. The calculation $\langle\hat{P}\rangle=P$ is complicated by the presence of the inverse operator in Eq. (4.12). It is instructive to consider the semiclassical approximation first, before proceeding to the exact calculation.

A. Semiclassical approximation

Suppose we approximate the inverse operator by writing

$$[S^{1/2}(S+1)^{1/2}+\hat{S}^z_n]^{-1}$$
$$\simeq[S^{1/2}(S+1)^{1/2}+\langle\hat{S}^z_n\rangle]^{-1} \ , \qquad (4.13)$$

which amounts to the drastic approximation

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

for all S. In the continuum limit we get

$$P=(\hbar S/a)\int_{-\infty}^{+\infty}dx\,(1-\cos\theta)(\partial_x\phi)$$
$$=(4\hbar S/a)\sin^{-1}(1-\alpha^2)^{1/2} \ , \qquad (4.14)$$

on using Eqs. (3.5) and (3.9). Thus $|P|\le 2\pi\hbar S/a$. We note that (4.14) is just the momentum of the classical soliton,[3] on identifying $S\hbar$ with $S_{\rm cl}$. Equations (4.7) and (4.14) lead to the dispersion relation

$$E(P)=(16JS^3\hbar)/|M|)\sin^2(Pa/4\hbar S) \ . \qquad (4.15)$$

In terms of the classical parameters, Eq. (4.15) reads

$$E(P)=(16J_{\rm cl}S^3_{\rm cl}/|M|)\sin^2(Pa/4S_{\rm cl}) \ , \qquad (4.16)$$

which is again the dispersion relation obtained in the classical case.[3] The mean-field-like approximation (4.13) evidently neglects quantum fluctuations in $\hat{S}^z_n$. This can be justified at best for the low-lying states of the system. Finally we observe that in this approximation, the group velocity of energy propagation,

$$C_g(P,M)=(\partial E/\partial P)_M \ , \qquad (4.17)$$

can be verified to be identical to the soliton velocity[19] v for all S.

B. Exact calculation

An exact calculation of P involves expanding

$$\hat{W}=[S^{1/2}(S+1)^{1/2}+\hat{S}^z_n]^{-1}$$

in powers of $\hat{S}^z_n$ and then calculating the relevant matrix elements of the operator products occurring in $\hat{P}$ term by term. It is readily seen that for a given S the expansion of the inverse operator contains powers of $\hat{S}^z_n$ up to $(\hat{S}^z_n)^{2S}$ only. The expansion coefficient are calculated[20] as follows: We set

$$\hat{W}=A_0+A_1\hat{S}^z+A_2(\hat{S}^z)^2+\cdots+A_{2S}(\hat{S}^z)^{2S} \ .$$

Then for a given S, we write down the diagonal matrix elements

$$\langle S_z = m | \hat{W} | S_z = m \rangle$$

of this equation, for the allowed values $m = S, S-1, \ldots, -S+1, -S$. This yields $2S$ simultaneous equations for the quantities $A_0, A_1, \ldots, A_{2S}$, which are easily solved. We thus obtain the following exact expressions for $\hat{W}$:

$$S = \tfrac{1}{2}: \quad \hat{W} = \sqrt{3} - 2\hat{S}_n^z , \tag{4.18a}$$

$$S = 1: \quad \hat{W} = (1/\sqrt{2}) - \hat{S}_n^z + (1/\sqrt{2})(\hat{S}_n^z)^2 , \tag{4.18b}$$

$$S = \tfrac{3}{2}: \quad \hat{W} = (5\sqrt{15}/42) - (5/21)\hat{S}_n^z + (2\sqrt{15}/21)(\hat{S}_n^z)^2 - \tfrac{4}{21}(\hat{S}_n^z)^3 . \tag{4.18c}$$

Substituting Eqs. (4.18) in Eq. (4.12) yields $\hat{P}$ for $S = \frac{1}{2}$, 1, and $\frac{3}{2}$, respectively. To calculate $P = \langle \hat{P} \rangle$, we need the expectation values $\langle (\hat{S}_n^z)^r \hat{S}_n^i \rangle$ and $\langle \hat{S}_n^i (\hat{S}_n^z)^r \rangle$, where $i = x, y$ and $r = 1, 2, \ldots, 2S$. The relevant matrix elements, evaluated by inserting complete sets of SCR states with the appropriate weight factors [see Eq. (2.7)] are listed in Appendix A. For large values of S (including $S = \frac{3}{2}$), random-phase approximation $\langle \hat{A}\hat{B} \rangle \simeq \langle \hat{A} \rangle \langle \hat{B} \rangle$ for any operators $\hat{A}$ and $\hat{B}$ is quite satisfactory. Carrying out the algebra (the essential steps of which are given in Appendix B), we finally obtain

$$\begin{aligned} Pa &= 2\sqrt{3}\hbar\alpha(1-\alpha^2)^{1/2} \quad (S = \tfrac{1}{2}) , \\ Pa &= 2\hbar\alpha(1-\alpha^2)^{1/2}(4.90 - 2.66\alpha^2) \quad (S = 1) , \\ Pa &\simeq 9\hbar\alpha(1-\alpha^2)^{1/2}[0.83 + 0.32(1-\alpha^2) \\ &\quad + 0.68(1-\alpha^2)^2 \\ &\quad + 0.88(1-\alpha^2)^3] \quad (S = \tfrac{3}{2}) . \end{aligned} \tag{4.19}$$

Figure 1 shows the variation of $(Pa/2\pi\hbar S)$ with α. Note that for each S there is a single maximum in P which shifts systematically towards the semiclassical limiting value $2\pi S\hbar/a$, as S increases. The semiclassical momentum given by Eq. (4.14) is also plotted for comparison. In contrast to the classical case, there are *two* values of α (and hence *two* possible soliton widths Γ) for each value of P.

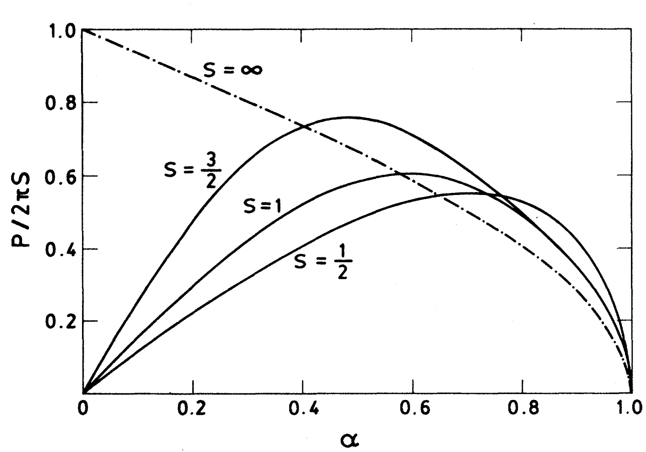

FIG. 1. The scaled momentum $P/2\pi S$ (in units of $\hbar a^{-1}$) vs α for $S = \frac{1}{2}$, 1, and $\frac{3}{2}$. The semiclassical momentum is given by the dot-dashed line.

V. SOLITON DISPERSION RELATION

By eliminating α between Eqs. (4.7) and (4.19) we obtain the dispersion relation for the solitons. (This can be done analytically for $S = \frac{1}{2}$.) The results are plotted in Fig. 2 for $S = \frac{1}{2}$, 1, and $\frac{3}{2}$, respectively, for a fixed value of $|M|$ (here set equal to unity for convenience). We have chosen different scales for the three cases so as to have the corresponding semiclassical spectra [Eq. (4.15)] coincide with each other, for ease of comparison. We see that the inclusion of quantum effects splits the spectrum for each S into two branches. Using Eq. (4.8), which connects the soliton energy and width, we conclude that the low-energy branch corresponds to large-width, spin-wave-like solitons, and the high-energy branch to narrow-width, particlelike excitations. The crossover occurs at a "critical" energy $E_c(S)$. It is clear from Fig. 2 that quantum corrections to the low-energy branch are relatively unimportant when compared to those for the upper branch. There is an S-dependent quantum cutoff momentum which is less than the semiclassical cutoff value $2\pi S\hbar/a$. As S increases, the lower branch increasingly dominates the spectrum, until it takes over completely in the classical limit ($S \to \infty$, $\hbar \to 0$).

The group velocity C_g [Eq. (4.17)] has opposite signs for the two branches, with $|C_g| \to \infty$ as $E \to E_c(S)$. This appears to be unphysical at first sight, but it is expected[21] that the excitation would become unstable if

$$|C_g| \geq v_{\max} = (4J\hbar^{-1}S\omega a^2)^{1/2}$$

(corresponding to $\alpha = 1$). This is based on a physical argument which suggests that energy transport cannot be associated with solitons in this regime. For $S = \frac{1}{2}$, we can show that this instability occurs for $(Pa/\hbar) \gtrsim 0.7$. For

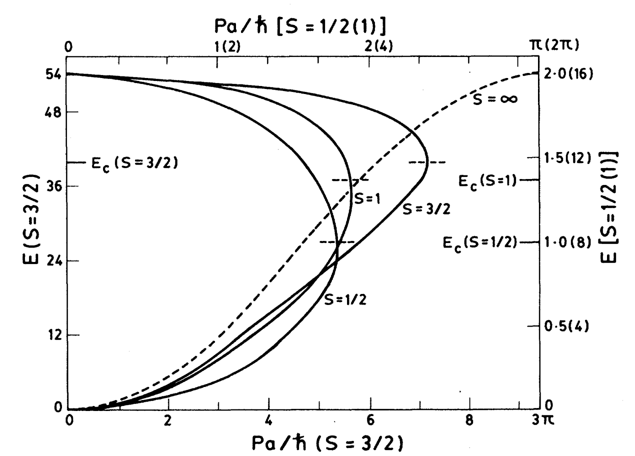

FIG. 2. Soliton energy E (in units of $J\hbar|M|^{-1}$) vs momentum P (in units of $\hbar a^{-1}$) for $S = \frac{1}{2}$, 1, and $\frac{3}{2}$. The numbers in parenthesis on the E and P axes indicate the scale for the case $S = 1$. The dashed line represents the semiclassical dispersion relation.

other spin values, numerical analysis is required to find the corresponding values of $(Pa/\hbar)$. If the foregoing heuristic reasoning is correct, we see from Fig. 2 that there is an intermediate range of energies (and widths) for which the solitons are unstable. Thus for low values of S, stable quantum solitons seem to exist only for small P. As S increases, the range of stability increases. It therefore appears that quantum fluctuations tend to affect the stability of the excitations quite significantly. Ignoring these fluctuations (i.e., the semiclassical approximation) simply yields $C_g = v$ for all S, implying that stable solitary waves occur for all P. We have not carried out a rigorous stability analysis of the quantum case; this is a heavy numerical problem in its own right.

We conclude this section with the following observations: It is known[18] that when a classical soliton solution in a continuous spin chain is quantized semiclassically, using a path integral method, its energy spectrum has the same form as the continuum limit of the exact multimagnon bound-state spectrum found by Bethe[22] for a discrete, *spin-*$\frac{1}{2}$ quantum chain, using his ansatz for the spin eigenstates. This interesting connection between the semiclassically quantized solitons of an integrable system and the bound states of the corresponding quantum system is obtained in other cases as well, such as the nonlinear Schrödinger and sine-Gordon field theories.[23] However, the validity of a semiclassical approximation is often questioned for spin systems with low S values. The method we have used shows how semiclassical expressions result when quantum fluctuations are neglected in certain operator expansions. We have also shown how quantum effects modify the classical soliton dispersion relation. As will be discussed in the next section, a semiclassical approximation can be strictly justified only for very large-width solitons. These observations and our results (Fig. 2) suggest that only such solitons—with *small amplitudes* and low energies—can be regarded as multimagnon bound states. This conclusion is physically realistic because, as is well known, magnons are also *small-amplitude,* low-lying excitations in a spin model.

VI. DISCUSSION

In this work we have studied the dynamics of solitons in a quantum Heisenberg ferromagnetic chain using a continuum approximation. This approximation is valid if the minimum width of a soliton is at least an order of magnitude larger than the nearest-neighbor distance in the chain. As seen from Eq. (3.6), this implies the requirement $(JS/\hbar\omega)^{1/2} \gtrsim 10$, providing a rough quantitative relationship between the parameters in the problem.

Figure 1 shows that quantum corrections to the soliton momentum are negligible for the large-width (low-energy) solitons, but are quite significant for the narrow-width (high-energy) solitons. This in turn leads to the two-branch dispersion relation for E versus P, given in Fig. 2. Recently, Haldane has questioned[24] the correctness of the conventional expression for the *classical* momentum [Eq. (4.10)] used extensively by earlier workers,[3,18] and hence also that of its quantum analog used by us[7] to obtain the two-branch spectrum. He has claimed[24] that the classical expression is not a true constant of motion because of the apparent singular behavior of the integrand when $S_z = -S$. However, it must be noted that since the single-soliton solution never takes on this singular value,[24] the expression is quite adequate for our study of quantum effects on *single*-soliton dynamics.

Haldane asserts[24] that in the spin-coherent-state approach, all the quantum corrections to the momentum will vanish identically, in the continuum model, to give $\langle \hat{P} \rangle = P_{sc}$, where P_{sc} is the semiclassical momentum obtained in Eq. (4.14). He therefore concludes that the dispersion relation must be identical (in functional form) to the classical one with a single branch,[3] and with the spin value S playing the role of a mere scale factor as in the classical case.

In this section, we first give a qualitative discussion which provides a physical interpretation of the two-branch spectrum. We then present a quantitative analysis to establish that Haldane's conclusions are incorrect. This is achieved by showing that certain mathematical steps used in the proof of the relationship $\langle \hat{P} \rangle = P_{sc}$ are invalid. However, in the course of our discussion, it will become clear that Haldane's general approach when properly carried out is not in conflict with our results, and indeed *further supports* our conclusion that a semiclassical approximation is satisfactory only for the low-energy, large-width solitons. (Details are given in Sec. VI B following.)

A. Breakdown of semiclassical approximation

Consider soliton dynamics for a fixed (finite) internal frequency ω. Note the simple relationship $E = |M|\omega$ for a solitary wave [Eq. (4.6)]. Thus its energy-frequency relation has the same form as that of any quantum, with $\hbar$ replaced by the constant of motion $|M|$. By direct analogy, Haldane[19] has suggested,

$$\lambda = 2\pi |M| / P \tag{6.1}$$

as the de Broglie wavelength of the soliton. Thus a semiclassical approximation is expected to break down when λ exceeds the width Γ of the soliton (wave packet).

Using Eqs. (4.5) and (4.14) in Eq. (6.1), we have

$$\lambda = a(JS/\hbar\omega)^{1/2} 2\pi (1-\alpha^2)^{1/2} / \sin^{-1}(1-\alpha^2)^{1/2} . \tag{6.2a}$$

The width is [Eq. (3.6)]

$$\Gamma = a(JS/\hbar\omega)^{1/2} (1-\alpha^2)^{-1/2} . \tag{6.2b}$$

It is easy to see that when $\alpha \to 1$, $\Gamma \to \infty$ and $\lambda \to 2\pi a (JS/\hbar\omega)^{1/2}$. Thus the semiclassical approximation is satisfactory for large-width, low-energy solitons. However, when

$$\alpha \to 0, \quad \Gamma = \lambda/4 = a(JS/\hbar\omega)^{1/2} .$$

Hence the quantum corrections must become more and more significant as α decreases. This explains the P versus α plot of Fig. 2. As α is decreased, Γ also decreases making the solitary wave more and more localized. This leads to an increase of the quantum-mechanical uncertainty in its momentum. Therefore the deviation of the quantum curve from the semiclassical (dashed) one must increase as α decreases. This can be achieved only if the quantum curve bends downwards, since the maximum quantum momentum cannot exceed the maximum semiclassical value $2\pi S\hbar/a$. Furthermore, a soliton with $\alpha\to 0$ corresponds to a minimum width, maximum (finite) amplitude, *particlelike* excitation with $v\to 0$ and $P\to 0$. Thus for each value of P, there result two types of solitary waves, one particlelike and the other spin-wave-like. The E versus P dispersion relation given in Fig. 2 can now be understood using similar arguments. As $E\to 0$, one notes that $\Gamma\to\infty$, with negligible quantum corrections at P_{sc}. However, an increase of energy leads to a decrease of the soliton width, with an accompanying enhancement in the quantum corrections to P_{sc}. Since the maximum quantum energy [Eq. (4.3)] is identical to the maximum value of the semiclassical energy, the dispersion curve *must* bend back, away from the semiclassical curve, leading to the two-branch spectrum described in Sec. V.

B. Proof that $\langle\hat P\rangle\neq P_{sc}$ in the spin-coherent approach

Next, let us consider the quantitative aspects of our result. Using the spin-coherent-state representation, we found that in the continuum approximation, the expressions for the total energy $E=\langle\hat H\rangle$ and the total angular momentum $M=\langle\hat M\rangle$ were identical to the semiclassical expressions. Unfortunately, the exact calculation of $\langle\hat P\rangle$ poses certain problems. *In principle,* it is possible to find $\langle\hat P\rangle$ by constructing an exact translation operator[24] for the discrete chain as

$$\hat T=\mathrm{Tr}[R(\hat S_1)R(\hat S_2)\cdots R(\hat S_N)] , \tag{6.3}$$

where $R(\hat S)$ is a $(2S+1)\times(2S+1)$ matrix operator, with a nontrivial dependence[25] on S. Then, since $\hat T=\exp(-i\hat P a/\hbar)$, one could formally determine $\langle\hat P\rangle$ using

$$\langle\hat P\rangle=+i(\hbar/a)\langle\ln\hat T\rangle . \tag{6.4}$$

However, as is obvious from Eq. (6.3), an explicit calculation of $\langle\ln\hat T\rangle$ is not an easy task. This was why, as a practical alternative, we adopted the ansatz (4.12) for $\hat P$. A systematic procedure for its construction is given in Sec. IV. (The ansatz follows logically from the correspondence principle.) We then calculated $\langle\hat P\rangle$ and found that $\langle\hat P\rangle\neq P_{sc}$. The conditions under which $\langle\hat P\rangle$ becomes P_{sc} were also discussed.

In what follows, we review Haldane's proof[24] of the relation $\langle\hat P\rangle\equiv P_{sc}$ and show that it is actually valid only for solitons whose width $\Gamma\to\infty$. To prove that $\langle\hat P\rangle=P_{sc}$, one must show that

$$i(\hbar/a)\langle\ln\hat T\rangle=P_{sc} \tag{6.5}$$

It is possible to write[24]

$$\begin{aligned}\langle\hat T\rangle&=\prod_n\langle\theta_n,\phi_n|\theta_{n-1},\phi_{n-1}\rangle\\&=\prod_n(\alpha_n^*\alpha_{n-1}+\beta_n^*\beta_{n-1})^{2S}\\&=\exp 2S\sum_n\ln(\alpha_n^*\alpha_{n-1}+\beta_n^*\beta_{n-1}) .\end{aligned} \tag{6.6}$$

Equation (6.6) can be easily verified by using Eq. (2.4) and defining

$$\alpha_n=\cos(\theta_n/2) ,$$

and

$$\beta_n=\sin(\theta_n/2)\exp(i\phi_n) .$$

In the continuum approximation, which is valid when the typical length scale of α and β (here the width of the soliton Γ) is $\gg a$, one is justified in writing [on using a scaled variable $x'=(x/\Gamma)$],

$$\alpha_{n-1}\to\alpha(x')-(a/\Gamma)\frac{\partial\alpha}{\partial x'}+O(a/\Gamma)^2 . \tag{6.7}$$

Then substituting Eq. (6.7) in Eq. (6.6) and using $\sum_n\to a^{-1}\int dx$ we get

$$\langle\hat T\rangle=\exp(2S/a)\Gamma\int dx'\ln\left[1-\left[\frac{a}{\Gamma}\right]\left[\alpha^*\frac{\partial\alpha}{\partial x'}+\beta^*\frac{\partial\beta}{\partial x}\right]+O\left[\frac{a}{\Gamma}\right]^2\right] . \tag{6.7a}$$

For $(a/\Gamma)\ll 1$ one may write

$$\ln\left[1-\left[\frac{a}{\Gamma}\right]\left[\alpha^*\frac{\partial\alpha}{\partial x}+\beta^*\frac{\partial\beta}{\partial x}\right]+O\left[\frac{a}{\Gamma}\right]^2\right]\simeq\left[\frac{-a}{\Gamma}\right]\left[\alpha^*\frac{\partial\alpha}{\partial x}+\beta^*\frac{\partial\beta}{\partial x}\right] . \tag{6.7b}$$

This leads to

$$\begin{aligned}\langle\hat T\rangle&=\exp(-2S)\int dx\left[\alpha^*\frac{\partial\alpha}{\partial x}+\beta^*\frac{\partial\beta}{\partial x}\right]\\&=\exp(iS)\int dx(\cos\theta-1)\left[\frac{\partial\phi}{\partial x}\right] .\end{aligned}$$

Thus on using Eq. (4.14) one gets

$$\langle\hat T\rangle=\exp(-iP_{sc}a/\hbar) . \tag{6.8}$$

This establishes that

$$i(\hbar/a)\ln\langle\hat T\rangle=P_{sc} . \tag{6.9}$$

However, a comparison of Eqs. (6.9) and (6.5) shows that, in order to prove that $\langle\hat P\rangle=P_{sc}$, one must also establish that

$$\ln\langle\hat T\rangle=\langle\ln\hat T\rangle \tag{6.10}$$

To do this, Haldane[24] defined a power series[25] expansion

$$\langle \ln\hat{T}\rangle = \sum_{l}^{\infty} C_l \langle \hat{T}^{\,l}\rangle ,$$

and similarly

$$\ln\langle \hat{T}\rangle = \sum_{l} C_l \langle \hat{T}\rangle^l .$$

One must then show that

$$\langle \hat{T}^{\,l}\rangle = \langle \hat{T}\rangle^l \text{ for all } l \tag{6.11}$$

in order to complete the proof of Eq. (6.10). However, as we shall see below, $\langle \hat{T}^{\,l}\rangle = \langle \hat{T}\rangle^l$ only for $l \ll (\Gamma/a)$ and not for all l.

Proceeding as in the case of Eq. (6.6), one writes[24]

$$\langle \hat{T}^{\,l}\rangle = \prod_n \langle \theta_n,\phi_n | \theta_{n-l},\phi_{n-l}\rangle$$
$$= \exp(2S) \sum_n \ln(\alpha_n^*\alpha_{n-l} + \beta_n^*\beta_{n-l}) . \tag{6.12}$$

(i) For $la \ll \Gamma$, one may write [analogous to Eq. (6.7)]

$$\alpha_{n-l} \rightarrow \alpha(x') - \left[\frac{la}{\Gamma}\right]\frac{\partial\alpha}{\partial x'} + O\left[\frac{la}{\Gamma}\right]^2 , \tag{6.13}$$

and follow the same steps as (6.7a) and (6.7b) with a replaced by la. The outcome is [see Eq. (14), Ref. 24]

$$\langle \hat{T}^{\,l}\rangle = \exp(-ilP_{sc}a/\hbar) \text{ for } la \ll \Gamma . \tag{6.14}$$

Combining Eqs. (6.8) and (6.4) gives

$$\langle \hat{T}^{\,l}\rangle = \langle \hat{T}\rangle^l \text{ for } la \ll \Gamma . \tag{6.15}$$

(ii) For $la > \Gamma$, Eq. (6.13) is obviously not valid, the higher-order terms becoming more important with increasing order. One must hence write, using Eq. (6.12),

$$\langle \hat{T}^{\,l}\rangle = \exp(2S/a)\Gamma \int dx' \ln\left[1 - \sum_n \left[\frac{la}{\Gamma}\right]^n \left[\alpha^* \frac{\partial^n\alpha}{\partial x'} + \beta^* \frac{\partial^n\beta}{\partial x'}\right]\right] . \tag{6.16}$$

The crucial step analogous to Eq. (6.7b), which led to (6.15), is invalid for $la > \Gamma$. Thus $\langle \hat{T}^{\,l}\rangle \neq \langle \hat{T}\rangle^l$ for $la > \Gamma$. Furthermore, the expression (6.16) shows that the calculation of $\langle \hat{T}^{\,l}\rangle$ is indeed nontrivial for $l > (\Gamma/a)$. It is possible to write

$$\langle \ln\hat{T}\rangle = \sum_{l<\Gamma/a} C_l\langle \hat{T}^{\,l}\rangle + \sum_{l\gtrsim(\Gamma/a)} C_l\langle \hat{T}^{\,l}\rangle ,$$

to yield

$$\langle \ln\hat{T}\rangle \simeq \ln\langle \hat{T}\rangle + \sum_{l\gtrsim(\Gamma/a)} C_l(\langle \hat{T}^{\,l}\rangle - \langle \hat{T}\rangle^l) . \tag{6.17}$$

Using Eqs. (6.4) and (6.9) in Eq. (6.17) yields

$$\langle \hat{P}\rangle \simeq P_{sc} + i(\hbar/a) \sum_{l\gtrsim(\Gamma/a)} C_l(\langle \hat{T}^{\,l}\rangle - \langle \hat{T}\rangle^l) . \tag{6.18}$$

For example, from Eq. (3.6), the minimum soliton width $\Gamma_{min} = (JS/\hbar\omega)^{1/2}a$. Thus if the internal frequency ω of the soliton is such that $\hbar\omega = JS/100$, and $\Gamma_{min} = 10a$ the continuum approximation Eq. (6.7) is valid.

Equations (6.8) and (6.16) may be used in Eq. (6.18) to write the correction $\langle \hat{P}\rangle - P_{sc}$ more explicitly, but its quantitative estimate is not very easy, lending support to the use of a good ansatz for $\hat{P}$ as we have done. However, certain qualitative conclusions can be drawn from Eq. (6.18).

(i) $\langle \hat{P}\rangle = P_{sc}$ when $\Gamma \rightarrow \infty$ $(E \rightarrow 0)$ showing that at sufficiently *low* energies the semiclassical and quantum dispersion relations coincide.

(ii) As Γ decreases, the correction increases, since more terms contribute in the summation over l. It is interesting to note that both these features have already been quantitatively exhibited in our results (Fig. 2). As the soliton energy increases and Γ decreases, quantum corrections become significant leading to the upper branch. As described earlier, this is to be expected, since, as the soliton becomes increasingly localized, the uncertainty in its momentum must increase, and this is what we find.

We parenthetically remark that the terminology *continuum limit* is conventionally used[4–7] in soliton literature in the sense of a continuum approximation $(a \ll \Gamma)$ to the underlying lattice model. However, in the foregoing discussion, even if one were interested in the strict continuum limit one has to take the limit $a \rightarrow o$ only *after* carrying out the integral in Eq. (6.16) (remembering that α and β also depend on a) and performing the l summation in Eq. (6.18), and our assertion holds.

We conclude with the following observations. In this work, we do not claim to have solved the full quantum-mechanical problem, which would involve not only the explicit construction of $\hat{T}$ but also an *exact* calculation of $\langle \ln\hat{T}\rangle$, using Eq. (6.3) to find $\langle \hat{P}\rangle$ in the spin-coherent representation. Since $\hat{T}$ has a nontrivial dependence[25] on S, this feature must appear in $\langle \hat{P}\rangle$ as well. It is encouraging that our ansatz leads to such a result, in addition to other conclusions that can be physically interpreted.

Calculations for the energy spectrum of Heisenberg Hamiltonians with other types of spin symmetries are underway.

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APPENDIX A

We list here the matrix elements that are used to calculate $P = \langle \hat{P}\rangle$ from Eq. (4.12). The site indices have been omitted, for simplicity of presentation.

The nondiagonal matrix elements of S^+ and S^z are found to be

$$\langle \theta,\phi|S^+|\theta',\phi'\rangle = 2S\tan(\theta'/2)\cos^{2S}(\theta'/2)\cos^{2S}(\theta/2)\exp(i\phi')F(\theta,\theta',\phi,\phi',S)$$

and

$$\langle \theta,\phi|S^z|\theta',\phi'\rangle = S\cos^{2S}(\theta'/2)\cos^{2S}(\theta/2)[1-\tan(\theta/2)\tan(\theta'/2)\exp i(\phi'-\phi)]F(\theta,\theta',\phi,\phi',S)\ , \tag{A1}$$

where

$$F(\theta,\theta',\phi,\phi',S) = [1+\tan(\theta/2)\tan(\theta'/2)\exp i(\phi'-\phi)]^{(2S-1)}\ .$$

Using (A.1) and the completeness relation Eq. (2.7), we find the following diagonal matrix elements:

(i) $S=\frac{1}{2}$:

$$\langle \theta,\phi|S^zS^+|\theta,\phi\rangle = \tfrac{1}{4}\sin\theta\exp(i\phi) = -\langle \theta,\phi|S^+S^z|\theta,\phi\rangle\ , \tag{A2}$$

(ii) $S=1$:

$$\begin{aligned}\langle \theta,\phi|S^zS^+|\theta,\phi\rangle &= \langle \theta,\phi|(S^z)^2S^+|\theta,\phi\rangle = 2\sin(\theta/2)\cos^3(\theta/2)\exp(i\phi)\ ,\\ \langle \theta,\phi|S^+S^z|\theta,\phi\rangle &= -\langle \theta,\phi|S^+(S^z)^2|\theta,\phi\rangle = -2\sin^{-3}(\theta/2)\cos(\theta/2)\exp(i\phi)\ ,\end{aligned} \tag{A3}$$

(iii) $S=\frac{3}{2}$ (the matrix elements needed in this case are as follows):

$$\begin{aligned}\langle \theta,\phi|(S^z)^2|\theta,\phi\rangle &= \tfrac{3}{2}\cos^2\theta+\tfrac{3}{4}\ ,\\ \langle \theta,\phi|(S^z)^3|\theta,\phi\rangle &= \tfrac{3}{4}\cos^3\theta+\tfrac{21}{8}\cos\theta\ .\end{aligned} \tag{A4}$$

APPENDIX B

We give here some of the intermediate steps leading to Eqs. (4.19) for P. (i) $S=\frac{1}{2}$: Substituting Eq. (4.18a) in Eq. (4.12) we obtain

$$P = (\hbar/4a)\left\langle \sum_n [(\sqrt{3}-2\hat{S}_n^z)(\hat{S}_n^x\hat{S}_{n+1}^y-\hat{S}_{n+1}^x\hat{S}_n^y)+(\hat{S}_n^x\hat{S}_{n+1}^y-\hat{S}_{n+1}^x\hat{S}_n^y)(\sqrt{3}-2\hat{S}_n^z)]\right\rangle\ . \tag{B1}$$

From Eq. (A2)

$$\langle \hat{S}_n^+\hat{S}_n^z+\hat{S}_n^z\hat{S}_n^+\rangle = 0\ . \tag{B2}$$

Using (B2) and Eq. (2.8) in Eq. (B1) yields

$$P = (\sqrt{3}\hbar/4a)\sum_n \sin\theta_n\sin\theta_{n+1}\sin(\phi_{n+1}-\phi_n)\ , \tag{B3}$$

which in the continuum approximation becomes

$$P = (\sqrt{3}\hbar/4a)\int_{-\infty}^{+\infty}\sin^2\theta(\partial_x\phi)dx\ . \tag{B4}$$

Equations (3.9) and (3.7) are used to write

$$P(S=\tfrac{1}{2}) = \sqrt{3}(\alpha\omega^{1/2}\hbar/a)\int_{-\infty}^{+\infty}\sin^2(\theta/2)dx\ . \tag{B5}$$

(ii) $S=1$: Substituting Eq. (4.18b) in Eq. (4.12) and simplifying, we get

$$\begin{aligned}P = (\hbar/2a)\Bigg\langle \Bigg[\sum_n \sqrt{2}(\hat{S}_n^x\hat{S}_{n+1}^y-\hat{S}_{n+1}^x\hat{S}_n^y)-(\hat{S}_n^z\hat{S}_n^x+\hat{S}_n^x\hat{S}_n^z)\hat{S}_{n+1}^y\\ +\hat{S}_{n+1}^x(\hat{S}_n^z\hat{S}_n^y+\hat{S}_n^y\hat{S}_n^z)+[(\hat{S}_n^z)^2\hat{S}_n^x+\hat{S}_n^x(\hat{S}_n^z)^2]\hat{S}_{n+1}^y-[(\hat{S}_n^z)^2\hat{S}_n^y+\hat{S}_n^y(\hat{S}_n^z)^2]\hat{S}_{n+1}^x\Bigg]\Bigg\rangle\ .\end{aligned} \tag{B6}$$

From Eq. (A3),

$$\begin{aligned}\langle \hat{S}_n^z\hat{S}_n^++\hat{S}_n^+\hat{S}_n^z\rangle &= \sin\theta_n\cos\theta_n\exp(i\phi_n)\ ,\\ \langle (\hat{S}_n^z)^2\hat{S}_n^++\hat{S}_n^+(\hat{S}_n^z)^2\rangle &= \sin\theta_n\exp(i\phi_n)\ .\end{aligned} \tag{B7}$$

Using Eq. (B7) in Eq. (B6) yields

$$P = (\hbar/2\sqrt{2a})\sum_n (3-\sqrt{2}\cos\theta_n)\sin\theta_n\sin\theta_{n+1}\sin(\phi_{n+1}-\phi_n)\ , \tag{B8}$$

which in the continuum approximation gives

$$P = (\hbar/2\sqrt{2a})\int_{-\infty}^{+\infty}\sin^2\theta(3-\sqrt{2}\cos\theta)(\partial_x\phi)dx\ . \tag{B9}$$

Once again, Eqs. (3.9) and (3.7) are used to obtain

$$P(S=1)=(\sqrt{2}\alpha\omega^{1/2}/a)\left[(3-\sqrt{2})\int_{-\infty}^{+\infty}\sin^2(\theta/2)dx+2\sqrt{2}\int_{-\infty}^{+\infty}\sin^4(\theta/2)dx\right] . \tag{B10}$$

(iii) $S=\frac{3}{2}$: While all the exact matrix elements occurring in P can be evaluated, the algebra becomes rather tedious. However, as explained in the text, the random-phase approximation is quite satisfactory in this case. We therefore set

$$\langle(\hat{S}_n^z)^r\hat{S}_n^x\rangle\simeq\langle(\hat{S}_n^z)^r\rangle\langle\hat{S}_n^r\rangle,\quad \text{etc., for } r=1,2,3 . \tag{B11}$$

Substituting Eq. (4.18c) in Eq. (4.12) and using (B11), we get

$$P=(\hbar/a)\sum_n(\langle\hat{S}_n^x\rangle\langle\hat{S}_{n+1}^y\rangle-\langle\hat{S}_n^y\rangle\langle\hat{S}_{n+1}^x\rangle)[\tfrac{5}{42}\sqrt{15}-\tfrac{5}{21}\langle\hat{S}_n^z\rangle+\tfrac{2}{21}\sqrt{15}\langle(\hat{S}_n^z)^2\rangle-\tfrac{4}{21}\langle(\hat{S}_n^z)^3\rangle] . \tag{B12}$$

Using Eqs. (2.8) and (A4) in (B12) and the continuum approximation gives

$$P(S=\tfrac{3}{2})\simeq(9\alpha\omega^{1/2}/a)\int_{-\infty}^{+\infty}[0.43\,\sin^2(\theta/2)+0.24\sin^4(\theta/2)+0.64\sin^6(\theta/2)+0.96\sin^8(\theta/2)]dx . \tag{B13}$$

The integrals appearing in P may be evaluated using the expression (3.5a), which leads to the following relationship:

$$\begin{aligned}\omega^{-1/2}&=\tfrac{1}{2}(1-\alpha^2)^{-1/2}\int_{-\infty}^{+\infty}\sin^2(\theta/2)dx=\tfrac{3}{4}(1-\alpha^2)^{-3/2}\int_{-\infty}^{+\infty}\sin^4(\theta/2)dx\\&=\tfrac{15}{16}(1-\alpha^2)^{-5/2}\int_{-\infty}^{+\infty}\sin^6(\theta/2)dx=\tfrac{35}{32}(1-\alpha^2)^{-7/2}\int_{-\infty}^{+\infty}\sin^8(\theta/2)dx .\end{aligned} \tag{B14}$$

Using, Eq. (B14) in (B5), (B10) and (B13), we obtain Eqs. (4.19).

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