Nonlinear excitations and their energy spectra in one-dimensional bilinearly coupled spin systems

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In this paper we have analyzed the problem of quantum energy spectra with antiferromagnetic bilinearly coupled spin chains of both integer and half-integer values. The method of analysis involved representing the Hamiltonian in second-quantized form followed by a derivation of quantum field equations of motion. These nonlinear equations were solved semiclassically and the subsequent quantum corrections provided criteria for the existence of gaps in the energy spectra. Our results confirm a conjecture of Haldane [Phys. Lett. **93A**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983); J. Appl. Phys. **57**, 3359 (1985)] with specific qualifications regarding the strength and next-nearest-neighbor spin-spin interactions.

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I. INTRODUCTION

In 1983 Haldane [1] suggested that antiferromagnetic quantum spin chains, where each spin is integer, have a finite energy gap in their spectrum whereas chains made up of half-odd-integer spins are gapless. Numerical studies were undertaken to try to confirm [2] that there was indeed a gap for chains with spins $S=1$. There were, however, at least initially, numerical convergence problems that clouded the issue and Bethe-ansatz-like approaches seemed to indicate that there might not be a gap when the spins were integral. In this latter approach, however, the interactions between the spins were not of the same form as those discussed by Haldane, so possibly like systems were not being compared. It should be mentioned that two decades earlier Lieb, Schultz, and Mattis [3] had provided a rigorous proof that there was no gap for half-odd-integer spins, but the method was shown to fail for integer spins. Spin wave theory for the simplest antiferromagnetic systems was developed by Anderson [4], Ziman [5], and Kubo [6] long ago and the situation was reviewed by Nagamiya, Yosida, and Kubo [7].

The Hamiltonian we shall use takes the standard form [8]

$$H=J_1\sum_{i=1}^{N}\mathbf{S}_i\cdot\mathbf{S}_{i+1}+J_2\sum_{i=1}^{N}\mathbf{S}_i\cdot\mathbf{S}_{i+2}\ . \tag{1.1}$$

That is, only interactions between nearest and next-nearest sites labeled i are incorporated, J_1 and J_2 being the corresponding coupling coefficients. We assume that there are N spins on the chain and we apply periodic boundary conditions at the ends, i.e., i-j is only a multiple of N when $i=j$.

Our intention in the present paper is to analyze the Haldane gap problem from a different perspective. To this end we shall employ recent quantum field theoretical advances that rely heavily on nonlinear analysis. The particular theoretical tool that will be used is called the method of coherent structures (MCS) [9,10]. In it the starting point is a second-quantized Hamiltonian containing both one-body and two-body terms. Subsequent calculations involve Heisenberg's equation of motion followed by a transformation to a quantum field representation. The final steps are based on a semiclassical approach where the classical component of the quantum field satisfies an integrable equation and the quantum component is found as a perturbation. It is important to emphasize that a topological argument plays a significant role in finding classical localized solutions and its quantum bound states. This, therefore, introduces similarities with the phenomenological Landau-Ginzburg (LG) model, but the level of approximation is much more reduced. Rather than describe the method itself in great detail, we refer the reader to Refs. [9,10] for a full exposition. The MCS approach will become very transparent as we systematically go through all the steps in the remainder of the paper and take the spin Hamiltonian of Eq. (1.1) as an example to study.

To briefly summarize the differences between the standard approaches to the problem and our method, we first of all must emphasize the nonlinear character of the quantum field that becomes manifest as a result of spin-spin interactions between lattice sites. A transition to a second-quantized formalism brings out the nonlinearity immediately and we see it in the emergence of both four- and six-legged terms in the equivalent Hamiltonian. To effectively deal with the problem of interactions (two- and three-quantum exchanges) we have decided to adopt the less popular route via quantum field equations of motion. The reason that such an approach has so far been less frequently adopted is most likely its inherent nonlinearity.

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However, we believe that nonlinearity is one of the key elements in the question of whether or not energy gaps exist in these spin chains. To circumvent the problems arising when a quantum formalism is inherently nonlinear, we subsequently adopt an approximation (which turns out to be fairly accurate) where the quantum field is assumed to comprise a large classical part and a quantum correction. This type of effect is commonly associated with coherent states and quantum phenomena that have macroscopic manifestations (e.g., superconductivity and superfluidity). In such cases a so-called field translation takes place with an attendant c-number component of the quantum field and hence a nonvanishing expectation value of the creation and the annihilation operators. This, of course, highlights a broken symmetry in the system and it is clearly so in the case of antiferromagnetic (AF) spin chains (translation symmetry emerges in the AF phase). We are also fortunate that the classical nonlinear field equations of motion can be solved analytically. We do so and then implement quantum corrections through a perturbation procedure developed in field theory mainly by Jackiw [17] and Rajaraman [21]. We apply this procedure to both spin-integer and half-integer cases separately since they call for different variants of the method. It turns out that the half-integer case is not invariant with respect to a full spin rotation at each site, which induces persistent phase currents in the chain interpolating between energetically equivalent spin configurations. This has serious implications on the available quantum bound states. In particular, in almost all half-integer cases the energy gap is removed since the classical envelope (localized solution of the field equation) is destabilized. As a result of this observation, we derive quantitative criteria for the existence of quantum gaps in the energy spectra of both spin integer and half-integer cases that are consistent with experimental results. In addition, our results confirm Haldane's conjecture with specific qualifications regarding the strength of nearest- and next-nearest-neighbor spin-spin interactions. Although the algebra is somewhat involved, we decided to omit many of its details for the reader's benefit since the approach presented here is quite different from the remaining body of literature on the topic. Once again, our overriding concern is with the role of nonlinearity, which leads to the emergence of stable, localized (semiclassical) structures within which quantum energy levels can be developed. The former can be thought of as effective potentials arising due to self-focusing in the system in analogy to other examples of self-focusing within the nonlinear Schrödinger equation hierarchy (e.g., optical fibers).

II. SECOND QUANTIZATION OF THE HAMILTONIAN

What we wish to do, in order to use the MCS, is to express the Hamiltonian of Eq. (1.1) in second-quantized form. We could opt to use fermion operators but, other than the spin-$\frac{1}{2}$ case, this seems to be unduly complicated for general half-integral spins. For example, we might write the spin component operators on each site i as

$$\begin{aligned} S_{zi} &= \sum_m m a_{im}^\dagger a_{im} \ , \\ S_{+i} &= \sum_m \sqrt{S(S+1)-m(m-1)}\, a_{im}^\dagger a_{i(m-1)} \ , \\ S_{-i} &= \sum_m \sqrt{S(S+1)-m(m+1)}\, a_{im}^\dagger a_{i(m+1)} \ , \end{aligned} \tag{2.1}$$

where the sum over m is over all the spin components $2S+1$ in number on one site [11]. If we adopted this approach, it would become necessary to introduce a field for each component and, furthermore, even though they satisfy SU(2) commutation rules on site, they commute between sites so a further transformation to other operators would become necessary to make them true fermion operators. Hence we shall use boson operators defined by the Holstein-Primakov [12] transformation, which is best understood as a particular case of a coupled Schwinger boson representation [13]. Thus we use

$$S_{zi} = S - b_i^\dagger b_i \ , \tag{2.2}$$

$$S_{+i} = S_{xi} + iS_{yi} = \sqrt{2S}\left[1-\frac{b_i^\dagger b_i}{2S}\right]^{1/2} b_i \ , \tag{2.3}$$

and

$$S_{-i} = S_{xi} - iS_{yi} = \sqrt{2S}\, b_i^\dagger \left[1-\frac{b_i^\dagger b_i}{2S}\right]^{1/2} . \tag{2.4}$$

In Eqs. (2.2)–(2.4) S is the total spin on each site and the z, x, and y components of spin are denoted by S_{zi}, S_{xi}, and S_{yi} for the spin on site i, respectively. The operators on each site b_i and $b_i^\dagger$ are Bose annihilators and creators. These operators already commute between sites and it is not now necessary to have labels for different components of spin, i.e., each operator is a creator or annihilator labeled with a site only. There are, however, disadvantages in that the Bose operators operate in a large-dimensional Hilbert space whereas the spin operators act only in a $(2S+1)$-dimensional space. In principle, therefore, we ought to introduce projectors so that the new operators are confined to the smaller of the two spaces (in fact, it is clear that when the eigenvalues of $b_i^\dagger b_i$ exceed $2S$, the root will become imaginary). It is usually unnecessary to do this as at low temperatures "spin deviations" (see Ref. [14], for example) are slight and $b_i^\dagger b_i/2S$ may be considered small. We shall therefore ignore this problem.

It should be mentioned that two other representations could be used. The first is the coupled fermion-drone system due to Jordan and Wigner [15], which has been discussed by Mattis [14]. Unfortunately, this would lead to two nonlinear coupled field equations and would be unnecessarily complicated. A second representation introduces Dyson operators [16] a_i ($a^\dagger$) so that

$$\begin{aligned} S_i^+ &= \sqrt{2S}\,[1-(a_i^\dagger a_i/2S)]a_i \ , \\ S_i^- &= \sqrt{2S}\, a_i^\dagger, \quad S_i^z = S - a_i^\dagger a_i \ . \end{aligned} \tag{2.5}$$

These operators overcome the problem of the square root that we have in a Holstein-Primakov representation, but this is at the expense of the Hamiltonian becoming non-

Hermitian and the transformation nonunitary, although the operators in Eq. (2.5) do satisfy the correct commutation rules. Thus we shall adhere to the operators in Eqs. (2.2)–(2.4) and note that the spin operators do satisfy the correct SU(2) commutation relations.

It may also be verified that the operators in Eqs. (2.2)–(2.4) also satisfy

$$\mathbf{S}_i\mathbf{S}_i = S_{zi}S_{zi} + \tfrac{1}{2}S_{-i}S_{+i} + \tfrac{1}{2}S_{+i}S_{-i} = S(S+1) \ . \tag{2.6}$$

Substituting the relations in Eqs. (2.2)–(2.4) in the Hamiltonian of Eq. (1.1) we obtain

$$\begin{aligned} H = J_1 \sum_{i=1}^{N} \Bigg[& (S - b_i^\dagger b_i)(S - b_{i+1}^\dagger b_{i+1}) \\ & + S b_i^\dagger \left[1 - \frac{b_i^\dagger b_i}{2S}\right]^{1/2} \left[1 - \frac{b_{i+1}^\dagger b_{i+1}}{2S}\right]^{1/2} b_{i+1} \\ & + S \left[1 - \frac{b_i^\dagger b_i}{2S}\right]^{1/2} b_i b_{i+1}^\dagger \left[1 - \frac{b_{i+1}^\dagger b_{i+1}}{2S}\right]^{1/2} \Bigg] \\ & + (\text{next-nearest-neighbor interaction}) \ . \end{aligned} \tag{2.7}$$

Note that Eq. (2.7) holds even for half-integral spins S despite the fact that these are fermions and we have used a bosonic second-quantized representation. The next problem is to tackle the awkward square roots that appear in Eq. (2.7). In order to use MCS in its simplest form we wish to retain only one-body- and two-body-like interaction terms, i.e., two-legged or four-legged operators only, respectively, since we want to retain only the first and simplest nonlinear term. There are at least three ways of doing this. These are as follows.

(a) Simply expand each square root and retain only the second term. Such a procedure seems a little naive since one would be truncating an infinite series with little hope of seeing how well retaining the second term would be.

(b) We could perform a so-called Maleev similarity transformation to rationalize the square roots. It does preserve the commutation rules and the on-site number operators [14], but because of its nonunitary character we will not adopt this.

(c) Suppose we denote the number operator $b_i^\dagger b_i$ by n and consider the eigenvalues of n for each value of S. From Eq. (2.2) we see that if $S = \frac{1}{2}$ then the eigenvalues of S_{zi} are $+\frac{1}{2}$ and $-\frac{1}{2}$ so the eigenvalues of n are those of $S - S_{zi}$, namely, $n = 0$ or 1. Similarly, if $S = 1$ the eigenvalues of n are 2,1,0 whereas when $S = \frac{3}{2}$ they will be 3,2,1,0. It may be shown that for any finite total spin S, the root operator may be written, for the eigenvalues at least, as a polynomial of order $2S$. That is

$$\left[1 - \frac{n}{2S}\right]^{1/2} = a_0 + a_1 n + a_2 n^2 + \cdots + a_{2S} n^{2S} \ , \tag{2.8}$$

where the above is understood to be a relation for the eigenvalues of n. For example, if the total spin $S = 1$, then

$$\left[1 - \frac{n}{2}\right]^{1/2} = 1 + \left[-\frac{3}{2} + \frac{2}{\sqrt{2}}\right] n + \left[\frac{1}{2} - \frac{1}{\sqrt{2}}\right] n^2 \ . \tag{2.9}$$

The first coefficient a_0 is always unity but all the coefficients $a_0, a_1, a_2, \ldots, a_{2S}$ may be found from a set of $2S+1$ linear equations, one for each eigenvalue, there being $2S+1$ coefficients $a_0, a_1, \ldots, a_{2S}$ to evaluate.

We shall take the coefficients appearing in Eq. (2.8) for each spin to be those in an expansion of each root n now being replaced, for example, in the nearest-neighbor interaction by $b_i^\dagger b_i$ or $b_{i+1}^\dagger b_{i+1}$ as appropriate. One advantage of this approach is that there is a finite number of terms, namely, $2S+1$, for each total spin S, so it is much easier to see whether the remainder terms are small relative to those retained. Furthermore, we eventually have to solve *classical* field equations so to insist that the eigenvalues of the operators from the roots are correct is not at all unreasonable. In Table I we list the coefficients $a_1, a_2, \ldots, a_{2S}$ for spins $S = 1, \frac{1}{2}, 1, \frac{3}{2}, \ldots, 10$. The one noticeable point to make about them is that a_1 for integral and half-integral spins is always negative. It is also obvious from Table I that the coefficients a_i rapidly decrease with increasing i, at least for small spin values, a useful feature in itself.

Using Eq. (2.8) and substituting into the Hamiltonian of Eq. (2.7) we find

$$\begin{aligned} H = J_1 \sum_{i=1}^{N} \{ & S^2 - S(b_i^\dagger b_i + b_{i+1}^\dagger b_{i+1} - b_i^\dagger b_{i+1} - b_{i+1}^\dagger b_i) \\ & + (b_i^\dagger b_i b_{i+1}^\dagger b_{i+1} + S a_1 b_i^\dagger b_{i+1}^\dagger b_{i+1} b_{i+1} + S a_1 b_{i+1}^\dagger b_{i+1}^\dagger b_{i+1} b_i + S a_1 b_i^\dagger b_i^\dagger b_i b_{i+1} + S a_1 b_{i+1}^\dagger b_i^\dagger b_i b_i) \\ & + (S a_2 b_i^\dagger b_{i+1}^\dagger b_{i+1} b_{i+1}^\dagger b_{i+1} b_{i+1} + S a_2 b_{i+1}^\dagger b_{i+1}^\dagger b_{i+1} b_{i+1}^\dagger b_{i+1} b_i + S a_1^2 b_i^\dagger b_i^\dagger b_i b_{i+1}^\dagger b_{i+1} b_{i+1} \\ & + S a_1^2 b_{i+1}^\dagger b_{i+1}^\dagger b_{i+1} b_i^\dagger b_i b_i + S a_2 b_i^\dagger b_i^\dagger b_i b_i^\dagger b_i b_{i+1} + S a_2 b_{i+1}^\dagger b_i^\dagger b_i b_i^\dagger b_i b_i) \} \\ & + (\text{next-nearest-neighbor terms}) \ , \end{aligned} \tag{2.10}$$

where we have written out six-legged operators explicitly. Some of these additional terms are *not* negligible and later we indicate how their effect may be included. At this point, however, we simply assume that the parameter a_1, which appears in Eq. (2.10), is an effective one. That we can view this parameter in this way, without affecting the form of the operators, becomes clear at a later stage. Clearly the next-nearest-neighbor term may be obtained from that for the nearest-neighbor interaction, given explicitly in Eq. (2.10) by the transformation

$$J_1 \to J_2, \quad b_i(b_i^\dagger) \to b_i(b_i^\dagger), \quad b_{i+1}(b_{i+1}^\dagger) \to b_{i+2}(b_{i+2}^\dagger) \ .$$

TABLE I. Coefficients appearing in the expansion of root operators in Eq. (2.8).

Spin	a_1	a_2	a_3	a_4	a_5	a_6	a_7	a_8	a_9	a_{10}	Sa_1
0.5	−1.0										−0.5
1.0	−0.085 79	−0.207 11									−0.085 79
1.5	−0.275 06	+0.139 31	−0.047 75								−0.412 59
2.0	−0.117 79	−0.023 77	+0.011 95	−0.004 36							−0.235 59
2.5	−0.119 38	+0.030 97	−0.025 93	+0.010 71	−0.001 94						−0.298 45
3.0	−0.093 78	+0.015 93	−0.014 40	+0.006 70	−0.001 78	+0.000 20					−0.281 33
3.5	−0.080 36	+0.015 61	−0.016 98	+0.011 55	−0.005 24	+0.001 41	−0.000 17				−0.281 25
4.0	−0.069 46	+0.012 77	−0.015 25	+0.012 24	−0.007 03	+0.002 71	−0.000 62	+0.000 07			−0.277 85
4.5	−0.061 15	+0.010 70	−0.013 93	+0.012 94	−0.009 06	+0.004 57	−0.001 56	+0.000 32	−0.000 03		−0.275 15
5.0	−0.054 54	+0.008 94	−0.012 36	+0.012 71	−0.010 23	+0.006 21	−0.002 74	+0.000 83	−0.000 15	+0.000 01	−0.272 70
5.5	−0.049 19	+0.007 49	−0.010 78	+0.011 85	−0.010 45	+0.007 20	−0.003 77	+0.001 44	−0.000 38	+0.000 06	−0.270 57
6.0	−0.044 79	+0.006 29	−0.009 21	+0.010 38	−0.009 46	+0.006 82	−0.003 80	+0.001 59	−0.000 48	+0.000 10	−0.268 72
6.5	−0.041 09	+0.005 29	−0.007 68	+0.008 37	−0.007 06	+0.004 30	−0.001 58	+0.000 02	+0.000 37	−0.000 24	−0.267 11
7.0	−0.037 96	+0.004 46	−0.006 21	+0.005 88	−0.003 07	−0.001 22	+0.004 63	−0.005 47	+0.004 11	−0.002 16	−0.265 71
7.5	−0.035 27	+0.003 76	−0.004 79	+0.002 95	+0.002 67	−0.010 68	+0.017 08	−0.018 34	+0.014 47	−0.008 58	−0.264 49
8.0	−0.032 93	+0.003 17	−0.003 43	−0.000 40	+0.010 33	−0.025 09	+0.038 60	−0.043 67	+0.037 92	−0.025 59	−0.263 42
8.5	−0.030 88	+0.002 66	−0.002 12	−0.004 13	+0.020 03	−0.045 54	+0.072 64	−0.088 48	+0.084 77	−0.064 51	−0.262 48
9.0	−0.029 07	+0.002 22	−0.000 87	−0.008 22	+0.031 94	−0.073 20	+0.123 32	−0.162 23	+0.170 66	−0.144 89	−0.261 64
9.5	−0.027 46	+0.001 84	+0.000 35	−0.012 69	+0.046 25	−0.109 50	+0.195 80	−0.277 62	+0.318 71	−0.298 96	−0.260 89
10.0	−0.026 02	+0.001 51	+0.001 54	−0.017 62	+0.063 50	−0.156 76	+0.297 75	−0.453 63	+0.565 09	−0.580 92	−0.260 22

Spin	a_{11}	a_{12}	a_{13}	a_{14}	a_{15}	a_{16}	a_{17}	a_{18}	a_{19}	a_{20}
5.5	0.000 00									
6.0	−0.000 01	0.000 0								
6.5	+0.000 08	−0.000 02	0.000 00							
7.0	+0.000 80	−0.000 20	+0.000 03	0.000 00						
7.5	+0.003 80	−0.001 22	+0.000 27	−0.000 04	0.000 00					
8.0	+0.013 37	−0.005 32	+0.001 56	−0.000 32	+0.000 04	0.000 00				
8.5	+0.038 94	−0.018 46	+0.006 74	−0.001 83	+0.000 35	−0.000 04	0.000 00			
9.0	+0.099 35	−0.054 69	+0.023 86	−0.008 07	+0.002 04	−0.000 36	+0.000 04	0.000 00		
9.5	+0.229 66	−0.144 02	+0.073 12	−0.029 62	+0.009 35	−0.002 22	+0.000 37	−0.000 04	0.000 00	
10.0	+0.494 48	−0.348 14	+0.201 67	−0.095 18	+0.036 03	−0.010 68	+0.002 39	−0.000 38	+0.000 04	0.000 00

Realizing that, by Eq. (2.5), Bose operators on different sites commute, we have used this to arrange the terms in Eq. (2.10) into pairs that are obviously the Hermitian conjugates of each other.

The next step in the analysis is to Fourier transform the second-quantized Hamiltonian of Eq. (2.10) so that we can directly use the methodology of the MCS and draw physical conclusions regarding the Hamiltonian's structure.

III. FOURIER TRANSFORMATION

We begin by Fourier transforming each annihilator and creator to remove the site dependence. Thus we set

$$b_j = N^{-1/2} \sum_{k=1}^{N} b_k \exp[+i\phi_k j] ,$$
$$b_j^\dagger = N^{-1/2} \sum_{k=1}^{N} b_k^\dagger \exp[-i\phi_k j] , \tag{3.1}$$

where the angles ϕ_k are defined by

$$\phi_k = \frac{2\pi k}{N} \quad \text{for } k = 1,2,\ldots,N \tag{3.2}$$

and the operators b_k and $b_k^\dagger$ satisfy Bose commutation rules.

Using Eq. (3.1) we see that

$$\sum_{j=1}^{N} (b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j)$$
$$= \frac{1}{N} \sum_{j=1}^{N} \sum_{k,l}^{N} b_k^\dagger b_l \exp\{-i[\phi_{kj} + \phi_l(j+1)]\} + \text{H.c.}$$
$$= \sum_{k=1}^{N} 2\cos(\phi_k) b_k^\dagger b_k \tag{3.3}$$

and similarly

$$\sum_{i=1}^{N} (b_i^\dagger b_{i+2} + b_{i+2}^\dagger b_i) = \sum_{k=1}^{N} 2\cos(2\phi_k) b_k^\dagger b_k . \tag{3.4}$$

Thus the one-body terms in Eq. (2.10) become

$$S^2 N(J_1 + J_2) + S \sum_{k=1}^{N} \{J_1[2\cos(\phi_k) - 2] + J_2[2\cos(2\phi_k) - 2]\} b_k^\dagger b_k , \tag{3.5}$$

where we have made use of translation invariance to obtain

$$\sum_{i=1}^{N} b_i^\dagger b_i = \sum_{i=1}^{N} b_{i+1}^\dagger b_{i+1} = \sum_{k=1}^{N} b_k^\dagger b_k .$$

In a very similar way we can find second-quantized forms for the two-body interactions and the truncated Hamiltonian becomes

$$H=S^2N(J_1+J_2)+2S\sum_{k=1}^{N}\{J_1[\cos(\phi_k)-1]+J_2[\cos(2\phi_k)-1]\}b_k^\dagger b_k$$
$$+\frac{1}{N}\sum_{k_1,k_2,k_3,k_4}^{N}(J_1\cos(\phi_{k_1}-\phi_{k_4})+J_2\cos2(\phi_{k_1}-\phi_{k_4})+2J_2Sa_1\{\cos[2(\phi_{k_2}-\phi_{k_3}-\phi_{k_4})]+\cos[2(\phi_{k_1}+\phi_{k_2}-\phi_{k_3})]\}$$
$$+2J_1Sa_1[\cos(\phi_{k_2}-\phi_{k_3}-\phi_{k_4})+\cos(\phi_{k_1}+\phi_{k_2}-\phi_{k_3})])\Delta(\phi_{k_1}+\phi_{k_2}-\phi_{k_3}-\phi_{k_4})b_{k_1}^\dagger b_{k_2}^\dagger b_{k_3}b_{k_4}\ . \quad (3.6)$$

We define

$$\omega_k=\{J_1[\cos(\phi_k)-1]+J_2[\cos(2\phi_k)-1]\}2S \quad (3.7)$$

and denote the coefficient of $b_{k_1}^\dagger b_{k_2}^\dagger b_{k_3}b_{k_4}$, apart from the $1/N$ factor, in Eq. (3.6) in the two-body term by Ω_{k_1,k_2,k_3}. The parameter $\Delta(\phi)$ is defined to be unity if $\phi=2\pi n$, where n is an integer or zero, and zero otherwise.

Therefore, we have accomplished a transformation from the original lattice type of Hamiltonian in Eq. (1.1) to a second-quantized wave number representation in the Hamiltonian of Eq. (3.4). The latter form, although seemingly more complex, is much more amenable to the subsequent analysis using the MCS. The next section provides the remaining steps in the quantum field theoretic investigation of this problem.

IV. EQUATIONS OF MOTION FOR THE QUANTUM FIELDS

Having obtained a suitable form of the Hamiltonian in Eq. (3.6) we then calculate the equation of motion of the particular Bose operator by using Heisenberg's equation of motion

$$i\hbar\partial_t b_\eta=-[H,b_\eta]_-\ . \quad (4.1)$$

For simplicity of exposition we write $k_1=k$, $k_2=l$, $k_3=m$, and $\Omega_{k_1,k_2,k_3,k_1+k_2-k_3}=\Omega_{klm}$, so the Hamiltonian H becomes

$$H=S^2N(J_1+J_2)+\sum_k\omega_k b_k^\dagger b_k+\sum_{k,l,m}\frac{\Omega_{klm}}{N}b_k^\dagger b_l^\dagger b_m b_{k+l-m}\ . \quad (4.2)$$

From the commutation rules we have

$$[b_k^\dagger b_k,b_{k'}]_-=-\delta_{kk'}b_k\ . \quad (4.3)$$

Similarly,

$$[b_k^\dagger b_l^\dagger b_m b_{k+l-m},b_{k'}]_-=-\delta_{k',l}b_k^\dagger b_m b_{k+l-m}-\delta_{k',k}b_l^\dagger b_m b_{k+l-m}\ . \quad (4.4)$$

Thus, from Eqs. (4.1)–(4.4) we have

$$i\hbar\partial_t b_{k'}=+\omega_k\delta_{k,k'}b_k+\sum_{k,l,m}\frac{\Omega_{klm}}{N}\{\delta_{k',l}b_k^\dagger b_m b_{l+k-m}+\delta_{k',k}b_l^\dagger b_m b_{l+k-m}\}\ , \quad (4.5)$$

where we have assumed that the conservation of momentum is satisfied. Both sides of Eq. (4.5) are now multiplied by $\exp(-i\bar{k}'x)$, divided by $\sqrt{N}$, and summed over k' from $k'=1$ to N. At the same time we define a quantum field

$$\psi(x)=N^{-1/2}\sum_{\bar{k}}b_{\bar{k}}\exp(-i\bar{k}x)\ , \quad (4.6)$$

where $\bar{k}$ is defined by $\bar{k}=2\pi k/N$. We are using a one-dimensional chain of spins so we define the field using $\exp[-i\bar{k}x]$ as opposed to the general situation where the exponential would be of the form $\exp[-i\bar{\mathbf{k}}\cdot\mathbf{r}]$. Furthermore, $\bar{\mathbf{k}}$ is regarded as a C number relative to b_k. Equation (4.5) now becomes

$$i\hbar\partial_t\psi=+\sum_{\bar{k}'=1}^{N}\frac{\omega_{\bar{k}'}}{\sqrt{N}}b_{\bar{k}'}\exp[-i\bar{k}'x]$$
$$+\sum_{\bar{k}',\bar{k},\bar{m}}\Omega_{\bar{k}\bar{k}'\bar{m}}\frac{b_{\bar{k}}^\dagger\exp(+i\bar{k}x)}{\sqrt{N}}\frac{b_{\bar{m}}\exp(-i\bar{m}x)}{\sqrt{N}}\frac{b_{\bar{k}'+\bar{k}-\bar{m}}^\dagger\exp[-i(\bar{k}'+\bar{k}-\bar{m})x]}{\sqrt{N}}$$
$$+\sum_{\bar{k}',\bar{l},\bar{m}}\Omega_{\bar{k}'\bar{l}\bar{m}}\frac{b_{\bar{l}}^\dagger\exp(+i\bar{l}x)}{\sqrt{N}}\frac{b_{\bar{m}}\exp(-i\bar{m}x)}{\sqrt{N}}\frac{b_{\bar{l}+\bar{k}'-\bar{m}}^\dagger\exp[-i(\bar{l}+\bar{k}'-\bar{m})x]}{\sqrt{N}}\ . \quad (4.7)$$

Since the two-body interaction in Eq. (4.2) may be written as

$$\frac{1}{N}\sum_{k,l,m}\Omega_{klm}b_k^\dagger b_l^\dagger b_m b_{k+l-m} \quad (4.8)$$

and as the annihilators and creators refer to bosons, we must have effectively

$$\Omega_{klm}=+\Omega_{lkm}\ . \quad (4.9)$$

Thus, in the second term of Eq. (4.7), using Eq. (4.9), we may set $\Omega_{\bar{k}\bar{k}'\bar{m}}=+\Omega_{\bar{k}'\bar{k}\bar{m}}$. Hence changing $\bar{l}$ to $\bar{k}$ in the third term of Eq. (4.7), our equation of motion becomes

$$i\hbar\partial_t\psi=\sum_{\bar{k}'=1}^{N}\frac{\omega_{\bar{k}'}}{\sqrt{N}}b_{\bar{k}'}\exp(-i\bar{k}'x)+2\sum_{\bar{k}',\bar{k},\bar{m}}\Omega_{\bar{k}'\bar{k}\bar{m}}\frac{b_{\bar{k}}^{\dagger}\exp[+i\bar{k}x]}{\sqrt{N}}\frac{b_{\bar{m}}\exp[-i\bar{m}x]}{\sqrt{N}}\times\frac{b_{\bar{k}'+\bar{k}-\bar{m}}^{\dagger}\exp[-i(\bar{k}'+\bar{k}-\bar{m})x]}{\sqrt{N}} \tag{4.10}$$

The procedure now in MCS is to take only the zeroth-order interaction terms. That is, we expand $\Omega_{k'lm}$ about a critical point in reciprocal space and retain only the zeroth-order term. We can make the specific assumption that, at this critical point, $\phi_k=\phi_{k'}=\phi_m=\phi_0$. We make the further assumption that ϕ_0 takes the value $\phi_0=0$ for a ferromagnetic ground state, $\phi_0=\pi$ for the antiferromagnetic case, and $0<\phi_0<\pi$ for the helicoidal structure. In other words, we identify the ground states of the various phases with a particular value of ϕ_k, for any k, namely, ϕ_0. The Ω's in Eq. (4.10) may therefore be taken out of the summation and, using the definition of the quantum field ψ in Eq. (4.6) and performing the summations, we find that the interaction term gives $\mu_3\psi^*\psi\psi$ where

$$\mu_3=2(J_1+J_2-2J_2\cos2\phi_0)\ . \tag{4.11}$$

In zeroth order, ω_k must be expanded to quadratic deviations from the critical point. The first and second derivatives of ω_k with respect to k are

$$\frac{d\omega_k}{dk}=\frac{2\pi}{N}\{-J_1\sin\phi_k-2J_2\sin2\phi_k\} \tag{4.12}$$

and

$$\frac{d^2\omega}{dk^2}=\left[\frac{2\pi}{N}\right]^2\{-J_1\cos\phi_k-4J_2\cos2\phi_k\}\ . \tag{4.13}$$

Thus,

$$\omega_k\approx2S[\mu_0+\mu_1(k-k_0)+\mu_2(k-k_0)^2]\ , \tag{4.14}$$

where

$$\mu_0=J_1(\cos\phi_0-1)+J_2(\cos2\phi_0-1)\ , \tag{4.15}$$

$$\mu_1=\frac{2\pi}{N}\{-J_1\sin\phi_0-2J_2\sin2\phi_0\}\ , \tag{4.16}$$

and

$$\mu_2=\frac{1}{2}\left[\frac{2\pi}{N}\right]^2\{-J_1\cos\phi_0-4J_2\cos2\phi_0\}\ . \tag{4.17}$$

Hence, using Eqs. (4.15)–(4.17) and (4.10), our equation of motion becomes

$$i\hbar\partial_t\psi=\hat{\mu}_0\psi+i\hat{\mu}_1\frac{\partial\psi}{\partial x}+\hat{\mu}_2\frac{\partial^2\psi}{\partial x^2}+\hat{\mu}_3\psi^{\dagger}\psi\psi\ , \tag{4.18}$$

where the coefficients are

$$\hat{\mu}_0=2S[J_1(\cos\phi_0-1)+J_2(\cos2\phi_0-1)]+\phi_0 2S(J_1\sin\phi_0+2J_2\sin2\phi_0)-S\phi_0^2(J_1\cos\phi_0+4J_2\cos2\phi_0)\ , \tag{4.19}$$

$$\hat{\mu}_1=2S\{-J_1\sin\phi_0-2J_2\sin2\phi_0\}-2S\{-J_1\cos\phi_0-4J_2\cos2\phi_0\}\phi_0\ , \tag{4.20}$$

$$\hat{\mu}_2=S\{+J_1\cos\phi_0+4J_2\cos2\phi_0\}\ , \tag{4.21}$$

and

$$\hat{\mu}_3=2\{J_1+J_2+4Sa_1J_1\cos\phi_0+4Sa_1J_2\cos2\phi_0\}\ . \tag{4.22}$$

Clearly Eq. (4.18) is of the nonlinear Schrödinger type and thus can be readily analyzed in the classical approximation, which we do in Sec. V. In Eq. (4.10), if we were to expand $\Omega_{\bar{k}'\bar{k}\bar{m}}$ to quadratic deviations from the critical point, we would find [9] contributions of the form

$$-2\left[\frac{\partial\psi^{\dagger}}{\partial x}\right]\psi\left[\frac{\partial\psi}{\partial x}\right]+i\left[\psi^{\dagger}\psi a\left[\frac{\partial\psi}{\partial x}\right]+\psi^{\dagger}a\left[\frac{\partial\psi}{\partial x}\right]\psi\right]+\left[\left[\frac{\partial^2\psi^{\dagger}}{\partial x^2}\right]\psi\psi+\psi^{\dagger}\psi\frac{\partial^2\psi}{\partial x^2}\right]\ ,$$

where a is a constant determined in terms of matrix elements of the original second-quantized Hamiltonian. In fact, a renormalization argument [9] may be used to show that these are the *only* terms we need to consider; all others redress the ones we retain. As these describe small deviations away from the critical point we omit consideration of these terms. However, we have retained quadratic deviations for ω_k since, apart from the zero order contribution μ_0 and the fact, as we see later, that the first derivative term may be removed, the quadratic term is the first nontrivial contribution to arise from the one-body component.

As commented earlier, below Eq. (2.10) we cannot simply drop other terms for the nearest-neighbor interaction other than those in Eq. (2.10). To see this we examine the six-legged terms that arise from nearest-neighbor coupling:

$$Sa_2b_i^{\dagger}b_{i+1}^{\dagger}b_{i+1}b_{i+1}b_{i+1}^{\dagger}b_{i+1}b_{i+1}+Sa_2b_{i+1}^{\dagger}b_{i+1}^{\dagger}b_{i+1}b_{i+1}b_{i+1}^{\dagger}b_{i+1}b_i+Sa_1^2b_i^{\dagger}b_i^{\dagger}b_ib_ib_{i+1}^{\dagger}b_{i+1}b_{i+1}+Sa_1^2b_{i+1}^{\dagger}b_{i+1}^{\dagger}b_{i+1}b_{i+1}b_i^{\dagger}b_ib_i+Sa_2b_i^{\dagger}b_i^{\dagger}b_ib_ib_i^{\dagger}b_ib_{i+1}+Sa_2b_{i+1}^{\dagger}b_i^{\dagger}b_ib_ib_i^{\dagger}b_ib_i\ . \tag{4.23}$$

By using the commutation relations for the annihilators and creators it is obviously possible to write them in the form $b^{\dagger}b^{\dagger}b^{\dagger}bbb$, the standard form of a second-quantized three-body operator. However, we find that when we do this two-body operators of the form $b^{\dagger}b^{\dagger}bb$ also appear and these will contribute to those in Eq. (2.10) and *also* will be of the *same order of magnitude* as those retained after the Fourier transformation in Eq. (3.1). The associated matrix ele-

ments for the three-body operators remaining are at least a factor of $1/N$ smaller so we can safely neglect them. From Eq. (4.10) it is clear that we shall obtain additional contributions

$$Sa_2 b_i^\dagger b_{i+1}^\dagger b_{i+1} b_{i+1} + Sa_2 b_{i+1}^\dagger b_{i+1}^\dagger b_{i+1} b_i + Sa_2 b_i^\dagger b_i^\dagger b_i b_{i+1} + Sa_2 b_{i+1}^\dagger b_i^\dagger b_i b_i \ , \tag{4.24}$$

the terms in a_1^2 being already in three-body form since annihilators and creators on different sites commute. By comparing Eq. (4.24) with Eq. (2.10) we see that each term or form of operator is modified by those in Eq. (4.24) by the addition of a_2 to a_1 to form an effective a_1. In fact, if we consider all other-legged operators we find that the effective a_1 becomes $a_{1\text{eff}}$, where

$$a_{1\text{eff}} = \sum_{r=0}^{2S} a_r \tag{4.25}$$

and the effective two-body coefficients become

$$\begin{aligned}\Omega_{k_1 k_2 k_3} = &(J_1 \cos(\phi_{k_1} - \phi_{k_4}) + J_2 \cos(\phi_{k_1} - \phi_{k_4}) + 2J_2 S a_{1\text{eff}} \{\cos[2(\phi_{k_2} - \phi_{k_3} - \phi_{k_4})] + \cos[2(\phi_{k_1} + \phi_{k_2} - \phi_{k_3})]\} \\ &+ 2J_1 S a_{1\text{eff}} [\cos(\phi_{k_2} - \phi_{k_3} - \phi_{k_4}) + \cos(\phi_{k_1} + \phi_{k_2} - \phi_{k_3})]) \Delta(\phi_{k_1} + \phi_{k_2} - \phi_{k_3} - \phi_{k_4})\end{aligned} \tag{4.26}$$

and three- and higher-body interactions are taken into account.

The corresponding three-body terms from Eq. (4.23) take the form

$$Sa_2 b_i^\dagger b_{i+1}^\dagger b_{i+1}^\dagger b_{i+1} b_{i+1} b_{i+1} + Sa_2 b_{i+1}^\dagger b_{i+1}^\dagger b_{i+1}^\dagger b_{i+1} b_{i+1} b_i \ , \tag{4.27a}$$

$$Sa_1^2 b_i^\dagger b_i^\dagger b_{i+1}^\dagger b_i b_{i+1} b_{i+1} + Sa_1^2 b_{i+1}^\dagger b_{i+1}^\dagger b_i^\dagger b_{i+1} b_i b_i \ , \tag{4.27b}$$

$$Sa_2 b_i^\dagger b_i^\dagger b_i^\dagger b_i b_i b_{i+1} + Sa_2 b_{i+1}^\dagger b_i^\dagger b_i^\dagger b_i b_i b_i \ , \tag{4.27c}$$

where the contributions are from nearest-neighbor couplings and have been arranged in Eq. (4.27) in Hermitian conjugate pairs. Utilizing Eqs. (3.1), the first term of Eq. (4.27a), for example, takes the form

$$\begin{aligned}+\frac{Sa_2}{N^3} \sum_{\substack{k_1,k_2,k_3 \\ k_4,k_5,k_6}} &\left[\sum_{j=1}^{N} \exp[i(-\phi_{k_1} - \phi_{k_2} - \phi_{k_3} + \phi_{k_4} + \phi_{k_5} + \phi_{k_6})j] \right] \\ &\times \exp[i(-\phi_{k_2} - \phi_{k_3} + \phi_{k_4} + \phi_{k_5} + \phi_{k_6})] \\ &\times b_{k_1}^\dagger b_{k_2}^\dagger b_{k_3}^\dagger b_{k_4} b_{k_5} b_{k_6} \ .\end{aligned} \tag{4.28}$$

The sum over j in Eq. (4.28) is only nonvanishing when

$$k_1 + k_2 + k_3 - k_4 - k_5 - k_6 = 0 \ ,$$

i.e., linear momentum is conserved, and produces a factor of N. The coefficients within the summation, since the exponentials have unit modulus, are less than or equal to unity. Similarly the other three-body terms have net coefficients of order $[S(a_2 \text{ or } a_1^2)/N^3]N$. Next-nearest-neighbor three-body interactions may be treated in an analogous way. Thus, by comparison with the two-body terms, the three-body contributions are a factor of $1/N$ smaller and may therefore be neglected.

V. CLASSICAL SOLUTION OF THE NLS

We begin by assuming that the dominant part of the quantum field ψ is classical in nature, but its quantum aspect can be subsequently recovered through semiclassical approximation [17]. We first assume $\psi(\mathbf{r})$ to be complex and remove the gradient term in Eq. (4.18) by changing the independent variable to a moving coordinate system, where

$$x \to x - (\hat{\mu}_1/\hbar)t \tag{5.1}$$

so that the equation of motion becomes

$$i\hbar \partial_t \psi = \hat{\mu}_0 \psi + \hat{\mu}_2 \frac{\partial^2 \psi}{\partial x^2} + \hat{\mu}_3 \psi^\dagger \psi \psi \ . \tag{5.2}$$

Next, we adopt a modulus-argument form for the field ψ and also introduce time dependence in the phase oscillations by writing

$$\psi(\mathbf{r},t) = e^{i\omega t} \eta(\mathbf{r}) \exp[i\phi(\mathbf{r})] \ . \tag{5.3}$$

This, when substituted into Eq. (5.2), results in two coupled equations for the real and the imaginary parts, respectively, giving

$$(\hat{\mu}_0 + \hbar\omega)\eta + \hat{\mu}_3 \eta^3 + \hat{\mu}_2 \nabla^2 \eta - \hat{\mu}_2 \eta (\nabla\phi)^2 = 0 \tag{5.4}$$

and

$$2\nabla\eta \cdot \nabla\phi + \eta \nabla^2 \phi = 0 \ . \tag{5.5}$$

It is easy to see that Eq. (5.5) can be thought of as a continuity equation since it is equivalent to

$$\frac{1}{\eta} \nabla \cdot [\eta^2 \nabla\phi] = 0 \tag{5.6}$$

and it can be directly integrated to give

$$\eta^2 \nabla\phi = \mathbf{C}_0 + \nabla \times \mathbf{F} \equiv \mathbf{j} \ , \tag{5.7}$$

where $\mathbf{C}_0$ is an arbitrary integration constant vector, $\mathbf{F}$ is an arbitrary vector function, and the right-hand side of Eq. (5.7) has been equated with a phase current density.

This latter quantity can be defined following standard quantum mechanical approaches as

$$\mathbf{j}=\tfrac{1}{2}\mathrm{Im}(\psi^*\nabla\psi-\psi\nabla\psi^*)\ . \tag{5.8}$$

We will see in a later section that it plays an important role in the Haldane gap phenomenon. With this definition and $\nabla\phi$ from Eq. (5.7) we return to Eq. (5.4) for the field envelope η and obtain an autonomous, effectively decoupled, differential equation in the form

$$(\hat{\mu}_0+\hbar\omega)\eta+\hat{\mu}_3\eta^3+\hat{\mu}_2\nabla^2\eta-\hat{\mu}_2\frac{j^2}{\eta^3}=0\ . \tag{5.9}$$

Let us first deal with the question of time-dependent oscillations. It is very easy to determine that the underlying Hamiltonian density giving Eq. (5.2), from the variational principle, is the celebrated LG Hamiltonian

$$H_{\mathrm{LG}}=\int dx\left[-\hat{\mu}_2|\nabla\psi|^2+\hat{\mu}_0|\psi|^2+\frac{\hat{\mu}_3}{2}|\psi|^4\right]\ . \tag{5.10}$$

With this functional it is also a simple task to show that both the mean-field (homogeneous) solutions to Eq. (5.9) and the higher energy localized solutions (which will be discussed shortly) increase their energy as ω is increased. Therefore, to obtain the lowest lying solutions we henceforth set $\omega=0$, meaning that stationary solutions are investigated in the first instance.

We now briefly discuss the solutions of Eq. (5.9) taking $j=0$ to begin with. This simplifies Eq. (5.9) further and brings us to consider a stationary nonlinear Klein-Gordon equation of the form

$$\hat{\mu}_0\eta+\hat{\mu}_3\eta^3+\hat{\mu}_2\frac{d^2\eta}{dx^2}=0 \tag{5.11}$$

in one-dimensional space. It can be immediately integrated to yield

$$\left[\frac{d\eta}{dx}\right]^2=\frac{-\hat{\mu}_3}{2\hat{\mu}_2}(\eta^2-\eta_1^2)(\eta^2-\eta_2^2)\ , \tag{5.12}$$

where $\mp\eta_1$ and $\mp\eta_2$ are the (possibly complex) roots of the quartic polynomial

$$\eta^4+\frac{2\hat{\mu}_0}{\hat{\mu}_3}\eta^2+c_0=P(\eta)\ , \tag{5.13}$$

where c_0 is an integration constant setting the energy scale. In our case, three types of real, nonsingular solutions can be readily found (see Fig. 1): (a) *constant* (homogeneous) solutions

$$\eta=\pm\eta_0=\pm(-\hat{\mu}_0/\hat{\mu}_3)^{1/2}\ , \tag{5.14}$$

which correspond to an antiferromagnetic ground state since the magnitude of the order parameter ψ can be interpreted as the sublattice magnetization; (b) *elliptic wave* solutions

$$\eta=\eta_1\mathrm{sn}[\pm\sqrt{\Delta}\eta_2(x-x_0),k] \tag{5.15}$$

where sn denotes a Jacobi elliptic function [18], $\Delta=-\hat{\mu}_3/2\hat{\mu}_2$, and the Jacobi modulus k is given by

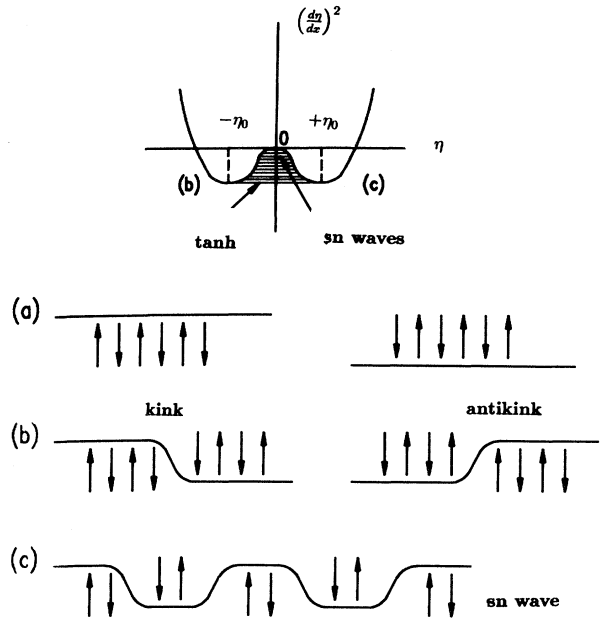

FIG. 1. Illustration of the real nonsingular types of solutions of Eq. (5.12): (a) constant, (b) domain walls, and (c) nonelliptic wave.

$k^2=\eta_1/\eta_2$ (in the limit of $k\to 1$ we obtain the following well-known localized solution below); and (c) a *domain wall* in the form

$$\eta=\pm\eta_1\tanh[\sqrt{\Delta}\eta_1(x-x_0)] \tag{5.16}$$

is found with x_0 denoting an arbitrary integration constant. It is apparent from Eq. (5.10), when the coupling constant for the cubic term is small, that for $\hat{\mu}_0/\hat{\mu}_2$ positive (this may happen when the gap disappears if r_0 is close to zero and below 0.25), the oscillatory solutions exist and similarly for (b) when $k\to 0$ [18]. Since $\hat{\mu}_3/\hat{\mu}_2$ is negative, the cubic term will have the effect of lowering the energy of the oscillatory solutions. In fact, it is easy to demonstrate that with the elliptic wave solutions in (b) above, when the elliptic modulus k tends to zero we obtain periodic solutions that have a higher energy than the solitonic form when $k\to 1$. That solitonic solutions may coexist with spin waves is very strongly supported by the recent work of Takeno and Kawasaki [19], who used a Dyson-Maleev transformation from spins to second-quantized operators, a coherent state ansatz, and a time-dependent variational principle [20] deduced equations of motion. They showed that there were two varieties of intrinsic self-localized models, symmetric and antisymmetric, below the magnon frequency band, which arose from the nonlinearity in magnon systems in one-dimensional Heisenberg antiferromagnets.

Turning now to the case when a nonzero current density $\mathbf{j}$ is present, we solve Eq. (5.9) in one-dimensional space and, as before, taking ω as a zero, to find the lowest energy solutions. This equation becomes

$$\hat{\mu}_0\eta+\hat{\mu}_3\eta^3+\hat{\mu}_2\frac{d^2\eta}{dx^2}-\frac{\hat{\mu}_2 j^2}{\eta^3}=0\ . \tag{5.17}$$

This can be readily integrated once to give

$$\left[\frac{d\eta}{dx}\right]^2=\Delta\left[\eta^4+\alpha\eta^2+\beta+\frac{\gamma}{\eta^2}\right]=R(\eta)\ , \tag{5.18}$$

where $\alpha=2\hat{\mu}_0/\hat{\mu}_3$, β is an arbitrary integration constant, and $\gamma=(2\hat{\mu}_2/\hat{\mu}_3)j^2$. Equation (5.18) can be analyzed in a way similar to Eq. (5.12) by plotting $(d\eta/dx)^2$ as a function of η. This is shown in Fig. 2. In this analysis it is crucial to determine the number and location of the extrema of the polynomial $R(\eta)$. Substituting $y=\eta^2$ reduces the problem to the cubic equation

$$2y^3+\alpha y^2-\gamma=0 \tag{5.19}$$

whose discriminant is proportional to

$$D=(\gamma^2/16)(-1+\alpha^3/27\gamma)\ . \tag{5.20}$$

It turns out that when

$$j<jc=\left[\frac{4}{27}\left|\frac{\hat{\mu}_0^3}{\hat{\mu}_2\hat{\mu}_3^2}\right|\right]^{1/2} \tag{5.21}$$

the polynomial $R(\eta)$ may have up to six real roots depending on the integration constant β. If, on the other hand, $j\geq j_c$ the cubic equation in (5.19) has only *one* real solution and consequently $R(\eta)$ has only *two real* roots. As illustrated in Fig. 2, the consequence is that, unlike in the $j<j_c$ case, when $j\geq j_c$ no nonsingular real solutions exist. For completeness we have summarized all the real solutions of Eq. (5.18) in Table II where the coefficients a, b, and c denote the roots of the cubic equation (5.19).

The solutions 1a and 1b are nonsingular and oscillate periodically via an elliptic sn function between the two

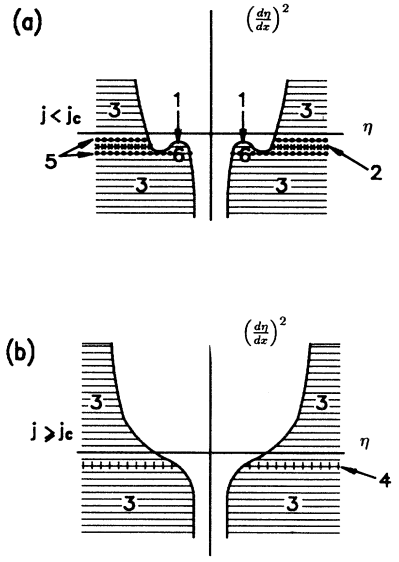

FIG. 2. Graphical analysis of the solutions to Eq. (5.18) for (a) $j<j_c$ and (b) $j\geq j_c$. The numbers indicated correspond to those in Table I.

real roots of the polynomial $R(\eta)$ as indicated in Table II. Solutions 2 and 3 are periodic and singular. Solution 4 is an algebraic singular function. Solution 5 is periodically singular, while solution 6 describes a localized solitary wave in the form of a "bump."

This completes the analysis of the classical solutions of the field equations of motion. What remains to be done is a semiclassical quantization, which we briefly discuss in Sec. VI.

TABLE II. Summary of the real solutions to Eq. (5.18) where a, b, and c denote the roots of Eq. (5.19), $y=\eta^2$, and k is the Jacobi modulus of the corresponding elliptic function.

No.	Root condition	Solution	g	k^2
1a	$a>b\geq y>c$	$\eta=\pm[c+(b-c)\mathrm{sn}^2(x/g,k)]^{1/2}$	$2/\sqrt{a-c}$	$(b-c)/(a-c)$
1b	$a>b>y\geq c$	$\eta=\pm\left[\frac{a(b-c)\mathrm{sn}^2(x/g,k)-b(a-c)}{(b-c)\mathrm{sn}^2(x/g,k)-(a-c)}\right]^{-1/2}$	$2/\sqrt{a-c}$	$(b-c)/(a-c)$
2	$y\geq a>b>c$	$\eta=\pm\left[\frac{(a-c)+\mathrm{csn}^2(x/g,k)}{\mathrm{sn}^2(x/g,k)}\right]^{-1/2}$	$2/\sqrt{a-c}$	$(b-c)/(a-c)$
3	$y\geq a$ $b,c\in C$	$\eta=\pm\left[\frac{(A-a)\mathrm{cn}(x/g,k)+(a+A)}{1-\mathrm{cn}(x/g,k)}\right]^{-1/2}$ $A^2=[(\mathrm{Re}b)-a]^2+(\mathrm{Im}b)^2$	$1/\sqrt{A}$	$\frac{A+(\mathrm{Re}b)-a}{2A}$
4	$y\geq a=b=c$	$\eta=\left[\frac{4+ax^2}{x^2}\right]^{1/2}$		
5	$y\geq a>b=c$	$\eta=\pm\left[a+(a-b)\tan\left\{\frac{x\sqrt{(a-b)}}{2}\right\}\right]^{1/2}$		
6	$c=b\geq y\geq a$	$\eta=\mp\left[a+(b-a)\tanh^2\left[\frac{x}{2}(b-a)\right]\right]^{1/2}$		

VI. SEMICLASSICAL QUANTIZATION

Let us recall that the initial field equation (5.2) was solved by assuming that the quantum field ψ is predominantly classical [17]. In this section we wish to examine the consequences of implementing semiclassical quantization carried out on the classical solutions through a linear perturbation procedure, i.e., we take

$$\psi=\psi_c+\Lambda\ , \tag{6.1}$$

where ψ is the quantum field, ψ_c its real classical component, and Λ the "small" quantum correction. Substituting Eq. (6.1) into Eq. (5.2) and linearizing with respect to Λ gives

$$\varepsilon\Lambda=\hat{\mu}_0\Lambda+3\hat{\mu}_3\psi_c^2\Lambda+\hat{\mu}_2\frac{d^2\Lambda}{dx^2}\ . \tag{6.2}$$

Note the presence of an effective potential proportional to ψ_c^2 as a result of a nonlinear classical envelope providing a binding potential. We will not engage in detailed discussions here since these can be readily consulted in monographs such as Rajaraman's book [21]. What has to be said, however, is a qualitative description of the problem. We therefore state the results for the types of classical solution ψ_c obtained in Sec. VI. First of all, constant solutions obviously lead to a continuum of plane waves in free space and no energy gaps are formed. If ψ_c is a singular solution, scattering states will be formed, but again no bound states with energy gaps arise. The third class of solution found in Sec. V are elliptic waves in which case the Schrödinger equation corresponding to Eq. (6.2) becomes a Lamé equation [22]. The characteristic feature is that energies associated with the solutions of this latter equation exhibit band formation. Although gaps may exist between bands, within a given band energies are distributed continuously.

The most important result from the above analysis is in regard to solitary wave solutions where ψ_c^2 is proportional to either the hyperbolic $(\tanh)^2$ or the $(\mathrm{sech})^2$ function. In both cases the Schrödinger equation can be reduced to the same general form where

$$\frac{-d^2\Lambda}{d\xi^2}+[(L^2-\omega_n^2)-L(L+1)\mathrm{sech}^2\xi]\Lambda=0 \tag{6.3}$$

with the independent variable ξ and the coefficient ω_c^2 being linearly transformed for convenience. In both cases the parameter $L=2$. In the language of Morse and Feshbach [23] $L(L+1)=v$ and $\omega_n^2-L^2=\epsilon-v$. With these parameters the bound energies are given by

$$\epsilon=\epsilon_n=v-[\sqrt{v+\tfrac{1}{4}}-(n+\tfrac{1}{2})]^2\ , \tag{6.4}$$

$$n=0,1,\ldots<\sqrt{v+\tfrac{1}{4}}-\tfrac{1}{2}\ . \tag{6.5}$$

As $L=2$ there are only *two* quantum bound states [22,23] corresponding to $n=1$ and 2 separated from a continuum above. The picture that then emerges is that the existence of localized sech or tanh solutions is a prerequisite for the presence of an energy gap conjectured by Haldane [1]. What we should do then is to examine our physical model presented in Secs. I–IV to see whether localized solutions for ψ_c are physically admissible. This is the objective of the next section.

VII. PHYSICAL INTERPRETATION

In order to obtain the tanh solution of Eq. (5.16) we must make sure that the asymptotic states $\mp\psi_0$, between which the solution interpolates and which correspond to the nonlinear potential's minima, are physically attainable. This means that not only must ψ_0 satisfy the equation of state

$$\hat{\mu}_0\psi_0+\hat{\mu}_3\psi_0^\dagger\psi_0\psi_0=0 \tag{7.1}$$

but it *must also* be compatible with the basic physical fact that the value of spin projection ranges from $-S$ to $+S$. Therefore, the field variable squared, i.e., $\psi_0^\dagger\psi_0$, must not exceed $2S$, which corresponds to a complete spin reversal from $-S$ to $+S$ on a single site. We therefore conclude that the following inequality must be satisfied if the two discrete quantum levels within the tanh envelope are to be of physical consequence. That is

$$|\psi_0|^2=\left|\frac{\hat{\mu}_0}{\hat{\mu}_3}\right|\leq 2S \tag{7.2}$$

if the chain's spectrum is to have a gap. To enable the reader to understand this we have schematically compared the two situations that arise in Fig. 3.

Let us now be more specific and interpret (7.2) in terms of our model parameters. Substituting $\hat{\mu}_0$ and $\hat{\mu}_3$ from Eqs. (4.19) and (4.22), respectively, and assuming the antiferromagnetic ground state, i.e., setting $\phi_0=\pi$, we obtain the criterion

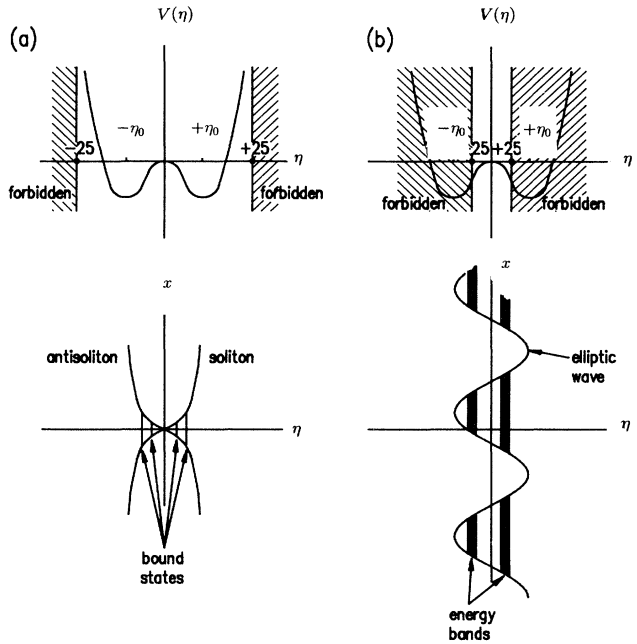

FIG. 3. Schematic illustration of the two possibilities in Eq. (7.1): (a) when $|\psi_0|^2<2S$ a soliton state is allowed that has two quantum bound states; (b) when $|\psi|^2>2S$ the soliton state is no longer physically admissible and a periodic solution with a continuum of quantum states within a band replaces the soliton.

$$\left| \frac{(4-\pi^2)+4\pi^2 r_0}{2\{(1-4Sa_1)+r_0(1+4Sa_1)\}} \right| \leq 2 , \tag{7.3}$$

where $r_0 = J_2/J_1$. First of all, in all the experimentally investigated materials the value of r_0 is very small indeed $r_0 \ll 1$ and hence the appropriate terms in Eq. (7.3) can be ignored. Second, using the values of Sa_1 from Table I, we find that the condition above is satisfied in the asymptotic limit of large spin S and on this basis we would expect the Haldane gap to be present there. Furthermore, all the lower spin values satisfy the above criterion. In the special case of $S=1$ the result of this analysis strongly depends on the value of r_0. It turns out that for $r_0 > 0.01$ the condition is satisfied and a gap exists. This latter result, however, has incorporated only a_1 in the inequality from Table I and has not included additional components to $a_{1\text{eff}}$ that arise from six-legged and higher-legged operators when the square root operators are expanded in Eq. (2.7). When the $a_{1\text{eff}}$ is used from Eq. (4.25), the above condition, i.e., that when $S=1, r_0 > 0.01$, is no longer applicable and Eq. (7.3) holds for all spin values S including $S=1$. However, it is interesting to note that even early numerical computations suffered from difficulties in the $S=1$ case, but from many later approaches so far reported a gap for the $S=1$ case appears to be certain.

On the basis of our analysis so far we could not account for the difference in behavior between integer and half-integer spin cases. However, an important distinction has to be taken into account when dealing with the half-integer cases. Here the local spin state is not invariant with respect to a 2π rotation, but results in a sign reversal unlike in the integer spin cases. Since a 2π rotation is not an invariant for the ground state of half-integral spins it induces a degeneracy that has to be accommodated by the system if time-reversal symmetry is not to be violated. Suppose the antiferromagnetic ground state of the spin chain begins at one end with a spin-up projection; then a completely equivalent arrangement beginning on a spin-down projection is allowed to exist. In order not to violate the time-reversal symmetry the spin chain will oscillate in time between these two equivalent ground states. This can be viewed as a flow of "phase current" backwards and forwards along the chain. The mathematical implications on the equation of motion are very simple to understand and this has been discussed from a more mathematical standpoint in the second part of Sec. V. We now use the results of Sec. V, which show that there exists a critical value of the current j_c for which all nonsingular solutions disappear (including the localized one). This value is given by the condition [see Eq. (5.21)]

$$-\hat{\mu}_2 j_c^2 = \frac{4}{27}\frac{\hat{\mu}_0^3}{\hat{\mu}_3^2} , \tag{7.4}$$

where

$$j_c = 2S\pi \tag{7.5}$$

since there exists a phase shift of π between adjacent spins in an antiferromagnetic state and since $\eta^2 \simeq 2S$ under the same conditions. The criterion in Eq. (7.4) translates into

$$\pi^2 = \frac{[-4-\pi^2(4r_0-1)]^3}{4\times 27(1-4r_0)\{1+r_0+4Sa_1(r_0-1)\}^2} , \tag{7.6}$$

which takes precedence over Eq. (7.3) for half-integer spin chains.

In Fig. 4 we have graphically illustrated the two generic situations for half-integer spins in regard to the value of the critical current density, i.e., (a) $j < j_c$, implying the existence of localized envelopes with two bound states (and hence an energy gap), and (b) $j \geq j_c$, where not only the bound states disappear but the classical envelope becomes delocalized removing the energy gap.

We have displayed the roots of the cubic in Eq. (7.6) for all spin values from $S=\frac{1}{2}$ to 10 in Table III from which it becomes clear that one root is always close to $r_0 \simeq +0.25$, one close to $r_0 \simeq +0.60$ and a negative root at $r_0 \simeq -0.46$. For lower values of spin these values depart from these latter values but the magnitude of the root is always greater than $|r_0| \simeq 0.21$. Bearing in mind that the term in r_0^3 from Eq. (7.5) can be chosen to be positive so that for large negative values of r_0 the cubic is negative and large positive values it is positive, we see that there will always be a regime where the gap disappears and this is between the negative root and the smallest positive root. Taking as an example the asymptotic value for Sa_1 of -0.25, for example, we can conclude that (a) the gap disappears (i.e., the current exceeds its critical value j_c) whenever

$$-0.42 \leq \frac{J_2}{J_1} = r_0 \leq +0.25 \quad \text{or} \quad \frac{J_2}{J_1} > 0.61$$

and (b) there may be a gap present (if the current density is less than j_c) for either

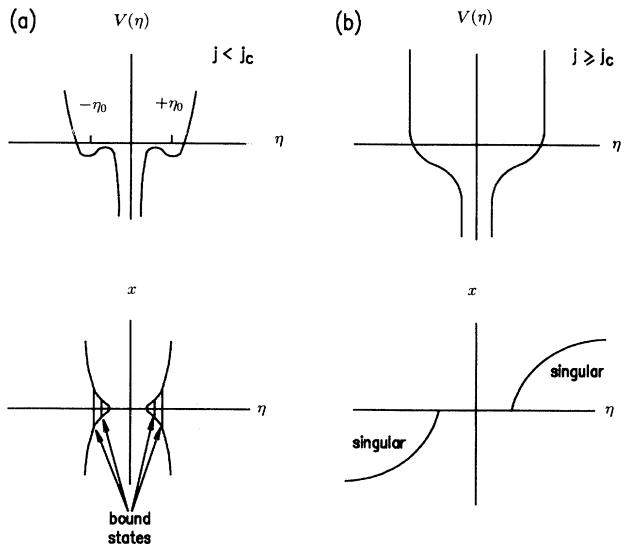

FIG. 4. Illustration of the effect of phase currents on the classical envelope and the quantum bound states within it.

TABLE III. Roots of Eq. (7.6) for different values of the spin S.

Spin			
0.5	+0.2476	+0.6994	−0.9331
1.0	+0.2582	+0.5303	−0.2104
1.5	+0.2526	+0.6719	−0.7187
2.0	+0.2544	+0.6083	−0.4011
2.5	+0.2536	+0.6336	−0.4997
3.0	+0.2538	+0.6270	−0.4715
3.5	+0.2538	+0.6270	−0.4714
4.0	+0.2539	+0.6256	−0.4659
4.5	+0.2539	+0.6246	−0.4616
5.0	+0.2538	+0.6237	−0.4577
5.5	+0.2539	+0.6228	−0.4543
6.0	+0.2540	+0.6220	−0.4515
6.5	+0.2540	+0.6214	−0.4489
7.0	+0.2540	+0.6208	−0.4467
7.5	+0.2540	+0.6203	−0.4448
8.0	+0.2540	+0.6199	−0.4432
8.5	+0.2540	+0.6196	−0.4417
9.0	+0.2540	+0.6192	−0.4404
9.5	+0.2540	+0.6189	−0.4392
10.0	+0.2540	+0.6186	−0.4381
$\rightarrow\infty$ $Sa_1=-0.25$	+0.2542	+0.6144	−0.4226

$$0.61>\frac{J_2}{J_1}=r_0>0.25 \quad \text{or} \quad \frac{J_2}{J_1}<-0.42 \ .$$

From Table III it is easily seen that similar conclusions hold for other values of spin. These conclusions are strongly supported by inserting values for $\hat{\mu}_0$, $\hat{\mu}_2$, and $\hat{\mu}_3$ from an exact treatment of the $S=\frac{1}{2}$ case [24] where here there is only one real root that is negative well away from the origin, the minimum in the cubic curve being above but close to the horizontal axis at $r_0\simeq 0.26$. As already mentioned, all the known experimental cases involve r_0 whose value is much less than one. Indeed, we recall that in the spin $S=\frac{1}{2}$ chain one of the criteria for antiferromagnetism [25] is that r_0 be less than 0.25. This then strongly indicates that the energy gap that appeared to exist based on Eq. (7.3) becomes forbidden as a result of the presence of phase currents whose densities exceed the critical value for all practical purposes. Thus we conclude that our analysis supports the Haldane theorem and we restate our findings in the following summary.

(a) For all integer spins there is an energy gap. This conclusion is without qualification and the apparent problem for $S=1$ may be eliminated when $Sa_{1\text{eff}}$ is used instead of Sa_1.

(b) For all half-integer spins the energy gap is absent as a result of phase currents, which can be seen as oscillations of the ground state in time between the equally allowed spin projections (see Fig. 4). A qualification we have to make here is that when J_2/J_1 exceeds the lowest positive root of the cubic in Eq. (7.6) and less than the largest positive root [this "window" varies (see Table II) with the value of spin, particularly for lower spin values] a gap may reemerge. A similar conclusion follows if r_0 is less than the negative root. Both these last situations, however, are most unlikely as r_0 is usually much less than 1, but we nevertheless encourage experimental studies in this direction.

In terms of the physical interpretation, the obtained analytical solutions to the equation of motion fall into three general classes. Nonsingular periodic solutions (elliptic waves) can be interpreted as nonlinear magnon waves (these are, for example, solutions Nos. 1a and 1b in Table II). Localized but nonsingular solutions, such as No. 6 in Table II, correspond to magnetic solitons formed in the chain. Singular solutions are less straightforward to interpret since they can either arise due to the various approximations taken in the procedure (e.g., the continuum limit) or they describe genuine defects in the magnetic structure of excitations. The existence of nonlinear magnons as well as magnetic solitons has been recently confirmed experimentally for the very representative AF compound $Ni(C_2H_8N_2)NO_2ClO_4$ (see Ref. [26]). Interestingly, it was commented there that the presence of an energy gap is related to a transition associated with a condensation effect of solitons. The latter can be limited by instanton fluctuations. These statements appear to closely echo our findings regarding the consequence of phase currents, which is the destruction of localized solutions.

VIII. DISCUSSION

Regarding the question of fully quantum mechanical treatments of Heisenberg or Ising metamagnetic chains, the reader is referred to Ref. [27] for an up-to-date review. However, it should be said that it has been known for a number of years now that the inclusion of next-nearest neighbors changes the nature of the ground state dramatically. While the quantum ground state is disordered in the nearest-neighbor case, a gap opens in the excitation spectrum of the next-nearest-neighbor model at a critical value of $j=J_2/J_1$. Simultaneously, ground-state correlations change from those governed by a power law to an exponential decay type [28,29]. The ground state, which is often referred to as the dimer phase, is characterized by the domination of short range, two-spin singlets, i.e., resonating valence bonds (RVB's). A comparison with the ground state of the classical Heisenberg model indicates that the RVB state appears in the helical phase [30]. The first rigorous example of a spin-one calculation for an antiferromagnetic chain with a Haldane phase was given by Affleck *et al.* [31], who showed that an $S=1$ isotropic bilinear-biquadratic spin chain has a short-range valence bond ground state with a gap in the infinite length limit. Moreover, Affleck, Lieb, and Kolb [32] showed that such a state does not appear in the spin half-integer case.

Exact, fully quantum mechanical calculations were, in the past, performed for several types of special cases. For example, for $J_2=0$ and $J_1/2$ the obtained results [33] indicate the absence of Néel long-range order. Instead, an ultrashort-range RVB has been found in the form as mentioned above. This RVB-type ground state seems to be also a characteristic feature of quantum Hamiltonians with bilinear and biquadratic exchange terms [31]. It therefore appears that quantum fluctuations destroy

long-range order arising due to the inherent nonlinearity of these problems. The extent to which this competition is resolved in favor of the disordering role of quantum fluctuations is not entirely clear and thus our results might be of use to this end. In fact, a number of papers have been published [34–36] that attack the problem starting from the classical limit (which is especially appropriate for spins larger than $\frac{1}{2}$) and then superimposing quantum corrections. It has been demonstrated that the emerging picture with thermally activated solitons works well in the low-temperature regime. A very recent paper [37], which came to the authors' attention after this paper was submitted for publication, applied a method very similar to ours to study nonlinear excitations in the antiferromagnetic CeAs. The authors applied the Dyson-Maleev transformation, a coherent state ansatz and a long-wavelength approximation. The results obtained there are similar to ours in it that the resultant equation is of a nonlinear Schrödinger type and it leads to soliton solutions representing bound magnon states. Their calculations, however, were restricted to the spin-$\frac{1}{2}$ case and did not directly attack the Haldane gap problem.

In connection with the question of soliton and solitary wave excitations in magnetic spin chains we refer the reader to a recent review paper by Mikeska and Steiner [38] for an exhaustive and up-to-date discussion. It should be mentioned, however, that within the classical framework, soliton solutions have been obtained [39,40] in the continuum limit of the Heisenberg model. Analogs of classical solitons have been found by various approximation techniques in quantum spin chains, too [41]. Quantum mechanically based approaches typically rely on coherent state representations and Holstein-Primakoff expansions for spin operators [42] and can also be used with the inclusion of biquadratic or anisotropic interaction terms [43]. The existence of solitons is intimately related to the integrability properties of the underlying models. Studies of quantum spin chains with competing bilinear and biquadratic interactions indicate that complete integrability can be furnished for spin chains with spins greater than one-half provided a suitable term in a power of $S_i S_j$ can be added to the Hamiltonian [44–46]. While soliton modes have been seen to exist and indeed govern the dynamics of elementary excitations in ferromagnetic Heisenberg-type Hamiltonians [47], much less progress has been evidenced in the antiferromagnetic cases. Some results have been obtained in classical isotropic Heisenberg antiferromagnetic spin chains [48] and evidence has been found of the presence of twists and instantons, which lock the neighboring spins into parallel pairs [49].

It appears therefore that our approach can be very useful since it allows for a consistent treatment of both integer and half-integer cases within a common scheme. The results we obtained point to the important role played by solitonlike excitations that lead to bound states with energy gaps. For spin half-integer cases, these localized states are subjected to phase currents that are similar to instantons that destabilize the bound state and close the energy gap. In this connection, Fadeejev and Takhtajan [50] showed that there exist integer spin models for arbitrary spin values S in which elementary excitations are spin-$\frac{1}{2}$ solitons with a dispersion relation independent of the spin magnitude S. The observable excitations are composite particles. For topological reasons solitons can only appear as singlet or triplet pairs. The energy of such soliton pairs is described by two parameters so that the excitations form a continuum spectrum. It has been very recently demonstrated that the symmetry properties of the excitation quanta are different for spin integer and half-integer cases [51], which is fully consistent with our results.

Finally, it should be said that the present approach can be applied to spin systems with the inclusion of distance-dependent interactions covering all "coordination spheres" and not just the nearest and the next-nearest neighbors. We intend to investigate this general case in the near future. A comparison then could be made with the fully quantum mechanical calculations of Pimpinelli [52], who showed that the RVB state remains the ground state even when the couplings between spins are extended to $2n$ next-nearest neighbors provided the relation $J_1 = 2n, J_2 = 2n-1, \ldots, J_{2n} = 1$ holds.

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