Semiclassical description of the frustrated antiferromagnetic chain

D. Allen and D. Sénéchal
Centre de Recherche en Physique du Solide et Département de Physique,
Université de Sherbrooke, Sherbrooke, Québec, Canada J1K 2R1
(Received 21 September 1994)

The antiferromagnetic Heisenberg model on a chain with nearest- and next-nearest-neighbor couplings is mapped onto the SO(3) nonlinear sigma model in the continuum limit. In one spatial dimension this model is always in its disordered phase and a gap opens to excited states. The latter form a doubly degenerate spin-1 branch at all orders in $1/N$. We argue that this feature should be present in the spin-1 Heisenberg model itself. Exact diagonalizations are used to support this claim. The inapplicability of this model to half-integer spin chains is discussed.

I. INTRODUCTION

Interest in low-dimensional magnetic systems has been great in recent years, partly because of the widespread belief that magnetism plays a key role in high-temperature superconductivity, but also because of the successful application of field-theoretic methods to these systems, in particular to spin chains. Indeed, a mapping from the spin-$s$ antiferromagnetic (AF) Heisenberg chain with nearest-neighbor (NN) coupling to the O(3)/O(2) $\sigma$ model has led Haldane to conjecture\textsuperscript{1} that integer spin chains should exhibit a gap to a triplet of excited states, whereas half-integer spin chains should not. This conjecture has later been confirmed by numerical calculations.\textsuperscript{2,3} Such a mapping may be termed \textit{semiclassical}, since it is constructed by introducing a local field characterizing the order parameter in the classical ground state and by taking into account fluctuations of the spin variables around this local order. In the case of the simple AF chain, a collinear order exists in the classical ground state and the local field introduced is a unit vector $\mathbf{e}(x,t)$ representing the staggered magnetization. The long-wavelength effective action obtained for this field is that of the O(3)/O(2) $\sigma$ model, with Lagrangian density

\begin{equation}
\mathcal{L}_\sigma = \frac{1}{2g} \left\{ \frac{1}{v} (\partial_t \mathbf{e})^2 - v(\partial_x \mathbf{e})^2 \right\} .
\end{equation}

The coupling $g$ and the velocity $v$ are related to the spin $s$, the AF coupling $J$, and the lattice spacing: $v = 2Jas$ and $g = 2/s$. To this action one must add a topological term $S_{\text{top}}$ for half-integer spin (cf. Sec. IV). An extension of this mapping to dimensions higher than 1 has been obtained by many authors, with the difference that no topological term arises, hence no distinction between half-integral and integral spin.

Dombre and Read\textsuperscript{4} have conducted a similar analysis for the antiferromagnetic Heisenberg model on a triangular lattice. The essential difference here is the presence of frustration, leading to a classical ground state characterized by a 120° order. The local order must then be specified by a rotation matrix instead of a unit vector and the order parameter is thus an element of SO(3). The long-wavelength action found in this case is the SO(3) nonlinear $\sigma$ model, with Lagrangian density

\begin{equation}
\mathcal{L} = \frac{1}{2g} \left\{ \frac{1}{v} \text{tr}(\partial_t R^{-1} \partial_t R) - v \text{tr}(P \nabla R^{-1} \cdot \nabla R) \right\} .
\end{equation}

Here $R(x,t)$ is a position- and time-dependent rotation matrix and $P$ is the constant diagonal matrix $\text{diag}[1,1,0]$. Again, the constants $g$ and $v$ depend on the spin $s$, the lattice spacing $a$, and the AF couplings $J$. At zero temperature and in dimension 2, this model has an ordered phase for $g < g_c$ and a disordered phase otherwise. Since $g \sim a/s$, the spin-$1/2$ case is the closest to the disordered phase. However, it is now widely believed\textsuperscript{5} that the ground state of the spin-$1/2$ antiferromagnet on a triangular lattice has long-range order and consequently the disordered phase of the SO(3) model is not physically realized in two-dimensional antiferromagnets, at least at half-filling (one spin per site).

In this work we will argue that this disordered phase of the SO(3) $\sigma$ model could be realized in a frustrated antiferromagnetic chain, with Hamiltonian

\begin{equation}
H = J \sum_n S_n \cdot S_{n+1} + J' \sum_n S_n \cdot S_{n+2} .
\end{equation}

Introducing a next-nearest-neighbor (NNN) coupling $J'$ modifies the classical ground state if $J'/J > \frac{1}{3}$: The spins still lie on a common plane, but instead of being collinear (as in the Néel state), they are arranged in a canted configuration (see Fig. 1) in which each spin makes an angle $\alpha$ with its predecessor, given by

\begin{equation}
\cos \alpha = -\frac{J}{4J'} .
\end{equation}

In the special case $J'/J = \frac{1}{3}$, the classical order is quite similar to that of the triangular lattice, with its 120° angle from site to site and its periodicity of three sites. For spin $\frac{1}{2}$ this particular case constitutes the Majumdar-Gosh model, whose ground state is exactly known.\textsuperscript{6} For
a generic value of $J'/J$ the classical order is incommensurable, with infinite periodicity. The spin-1 case has been studied previously using various methods: exact diagonalizations\textsuperscript{7} and approximate mappings to field theories involving fermions\textsuperscript{8} or bosons,\textsuperscript{9,10} among others.

This paper is organized as follows. In Sec. II we explain how to obtain the SO(3) nonlinear $\sigma$ model as the continuum limit of the model defined in Eq. (3). In Sec. III we argue that the disordered phase of this model is characterized by a singlet ground state with a gap to two degenerate triplets of excited states. Hence this model cannot adequately represent the half-integer NNN chain, but may be correct for integer spin. In Sec. IV we discuss our results with the help of exact diagonalization results and discuss the apparent lack of distinction between integer and half-integer spin in this model.

\section*{II. SEMICLASSICAL MAPPING TO THE SO(3) NONLINEAR $\sigma$ MODEL}

In this section we argue that the long-wavelength, continuum theory describing the frustrated antiferromagnetic chain is specified by the Lagrangian density of Eq. (17), with the notation explained thereafter.

The Lagrangian description of spin dynamics, as used in path integrals, requires the introduction of spin coherent states. The unfamiliar reader is referred to Fradkin's text\textsuperscript{11} or to Manousakis' review.\textsuperscript{12} Each quantum spin $S_i$ is described by a fluctuating unit vector $\mathbf{n}_i$ and the action associated to a spin Hamiltonian $H$ is

$$ S = \int dt \left\{ s \sum_i A(\mathbf{n}_i) \cdot \partial_t \mathbf{n}_i - H \right\}, \quad (5) $$

wherein $S_i$ is replaced by $s\mathbf{n}_i$ in the Hamiltonian. $A$ is the vector potential of a magnetic monopole of flux $4\pi$. Thus, given a closed curve $\mathbf{n}(t)$ on the unit sphere, the integral $\int A \cdot d\mathbf{n}$ equals the area of the sphere enclosed by the curve, modulo $4\pi$.

We shall use a description of each spin $S_i$ in terms of a slowly varying SO(3) order parameter $R(x, t)$ and a local magnetization vector $\mathbf{l}(x, t)$:

$$ S_i = \frac{s R(n_i^x + a l)}{|n_i^x + a l|}, \quad (6a) $$

$$ n_i^x = i \cos(kx) + j \sin(kx). \quad (6b) $$

Here $n_i^x$ is the orientation of the spin $S_i$ in a classical ground state taken as reference, in which all spins lie on the plane defined by two mutually orthogonal unit vectors $i$ and $j$; $\alpha$ is the pitch of this ground state, as given in Eq. (4); finally, $a$ is the lattice spacing: It is assumed that the spin configurations that contribute significantly to the path integral are locally close to the classical ground state, and the approximation that the deviation $a\mathbf{l}$ is small will be controlled at the same time as the continuum approximation.

Some comments are in order concerning this representation. If $J' = J/2$ (or $\alpha = 2\pi/3$), the periodicity is 3 and the relation (6) may be considered as a \textit{bona fide} change of variables if we group the spins in sets of 3 and assume that the fields $R$ and $\mathbf{l}$ do not vary within such sets. We check that the number of degrees of freedom match: six per set of three spins. However, it is more convenient to assume that $R$ and $\mathbf{l}$ vary slowly from site to site, in which case the representation (6) may not be regarded as a change of variables, but simply as long-wavelength description of the fluctuations around the classical ground state; then we need not restrict ourselves to the case $J' = J/2$.

The next step is to substitute the representation (6) into the action (5) and to Taylor expand when needed in order to get a continuum action in terms of $R$ and $\mathbf{l}$ only. We will treat the kinetic term first, and then the Hamiltonian. For the sake of convenience, we will assume a periodicity of $N$ spins in the classical ground state. The case $N = 3$ (or $J' = J/2$) is the simplest, leading to a calculation almost identical to that of Ref. 4. The next simplest is $N = 5$, with $J' \approx 0.809J$, and so on.

An explicit calculation of the kinetic term is not needed here, since it would be almost identical to that of Ref. 4, to which the reader is referred. The difference here lies in the number of reference vectors $n_i^x$, which is $N$ instead of 3. The kinetic part of the Lagrangian density is then

$$ L_K = s(T\mathbf{l}) \cdot \mathbf{V}, \quad (7) $$

with the definitions

$$ T_{ab} = \delta_{ab} - \langle n_i^a n_i^c \rangle \left( \begin{array}{ccc} 1 & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{array} \right), \quad (8a) $$

$$ V_a = -\frac{1}{2} \epsilon_{abc} (R^{-1} \partial_t R)_{bc}, \quad (8b) $$

wherein the indices in spin space correspond to the axes defined by $i$, $j$, and $i \times j$, and $\langle \cdots \rangle$ means an average over $N$ contiguous sites. In order to write down the continuum limit of the Hamiltonian $H$, we need to calculate the interaction $H^{(k)}$ of a spin $S_k$ with its four neighbors and then average the result over the $N$ spins $S_k$ of the period. Specifically, the Hamiltonian density is

$$ H = \frac{1}{2aN} \sum_k H^{(k)} = \frac{1}{2a} \langle H^{(k)} \rangle, \quad (9) $$
The contribution $H^{(k)}$ may be written as follows:

$$H^{(k)} = J \left\{ S_k \cdot S_{k+1} + S_k \cdot S_{k-1} + \frac{J'}{J} S_k \cdot S_{k+2} + \frac{J'}{J} S_k \cdot S_{k-2} \right\}$$

$$+ a J \left\{ S_k \cdot \partial_z S_{k+1} - S_k \cdot \partial_z S_{k-1} + \frac{2J'}{J} S_k \cdot \partial_z S_{k+2} - \frac{2J'}{J} S_k \cdot \partial_z S_{k-2} \right\}$$

$$+ \frac{a^2 J}{2} \left\{ S_k \cdot \partial_z^2 S_{k+1} + S_k \cdot \partial_z^2 S_{k-1} + \frac{4J'}{J} S_k \cdot \partial_z^2 S_{k+2} + \frac{4J'}{J} S_k \cdot \partial_z^2 S_{k-2} \right\} + \cdots,$$  \hspace{1cm} (10)

where the spin $S_n$ stands in fact for its expression in terms of $R$ and $l$ \cite{6} and where the derivatives act on these same fields. We will carry the expansion to second order only, enough to yield a nontrivial Lagrangian. We shall also use a Taylor expanded version of the representation (6):

$$S_n = s R_2 (n_n^c) + sa R (l - [l \cdot n_n^c]) n_n^c$$

$$+ sa R (n_n^c) \left[ \frac{1}{2} (n_n^c \cdot l)^2 - \frac{1}{4} l^2 \right]$$

$$- sa R (l) [n_n^c \cdot l] + O(a^3).$$  \hspace{1cm} (11)

We may then write the Hamiltonian density as an expansion in powers of $a$:

$$\mathcal{H} = \mathcal{H}^{(0)} + a \mathcal{H}^{(1)} + a^2 \mathcal{H}^{(2)} + \cdots.  \hspace{1cm} (12)$$

$\mathcal{H}^{(0)}$ is a constant, independent of $R$ and $l$. $\mathcal{H}^{(1)}$ vanishes for the following reasons: Part of it depends on $l$, but it is proportional to $\langle n_n^c \rangle$, which is zero. Another part depends on $R$, and is given by

$$\mathcal{H}^{(1)} = \frac{s^2}{2a} R^{-1} \partial_z R \left\{ J \langle n_{k,a} n_{k+1,b}^c \rangle - \langle n_{k,a} n_{k-1,b}^c \rangle \right\}$$

$$+ 2J' \langle n_{k,a} n_{k+2,b}^c \rangle - \langle n_{k,a} n_{k-2,b}^c \rangle \}.$$  \hspace{1cm} (13)

But one easily calculates that

$$\langle n_{k,a} n_{k+n,b}^c \rangle = \frac{1}{2} \begin{pmatrix} \cos \alpha & \sin \alpha & 0 \\ -\sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$  \hspace{1cm} (14)

After substituting and using the relation (4), we find out that the expression (13) vanishes.

Finally, we are left with the second-order part $\mathcal{H}^{(2)}$. It is a straightforward exercise to show that

$$\mathcal{H} = \frac{J a s^2}{2} I_a M_{ab} I_b - \frac{J a s^2}{4} \left( \xi - \frac{1}{\xi} \right) \text{tr}[P \partial_z R^{-1} \partial_z R],$$  \hspace{1cm} (15)

where $\xi = -\cos \alpha = J/4J'$ and where the diagonal matrix $M$ has elements

$$M_{33} = \frac{(1 + \xi)^2}{\xi}, \hspace{0.5cm} M_{11} = M_{22} = M_{33}(\xi^2 - \xi + \frac{1}{2}).$$  \hspace{1cm} (16)

Again, the matrix $P$ is the projector onto the plane defined by $I$ and $J$, as in Eq. (2). The full Lagrangian density is then $\mathcal{L} = \mathcal{E}_K - \mathcal{H}$.

The last step consists in integrating out the field $I$. Since the latter appears quadratically in $\mathcal{L}$, this operation amounts to substituting into $\mathcal{L}$ the solution of the classical equations of motion for $I$. The final result for the Lagrangian density is

$$\mathcal{L} = \frac{1}{2 \tilde{g}} \left\{ \frac{1}{\tilde{c}} \text{tr}[Q \partial_z R^{-1} \partial_z R] - \tilde{c} \text{tr}[P \partial_z R^{-1} \partial_z R] \right\},$$  \hspace{1cm} (17)

where the matrix $Q$ is diagonal, with elements

$$Q_{11} = Q_{22} = 1, \hspace{1cm} Q_{33} = \frac{2\xi(1 - \xi)}{\xi^2 + (\xi - 1)^2},$$  \hspace{1cm} (18)

and where the constants $\tilde{g}$ and $\tilde{c}$ are defined as

$$\tilde{g} = \frac{2}{s} \sqrt{\frac{1 + \xi}{1 - \xi}},$$  \hspace{1cm} (19a)

$$\tilde{c} = J a s \frac{1 + \xi}{\xi} \sqrt{1 - \xi^2}. $$  \hspace{1cm} (19b)

In the special case $\xi = \frac{1}{2}$, which corresponds to $J' = J/2$ and $\alpha = 2\pi/3$, one recovers precisely the form of the Lagrangian (2) since $Q_{33} = 1$. The parameter $\xi$ ranges from 0 ($J' \to \infty$) to 1 ($J' = J/4$). The characteristic speed $\tilde{c}$ diverges as $\xi \to 0$, whereas the coupling constant $\tilde{g}$ diverges as $\xi \to 1$, the collinear phase boundary. In all cases, the Lagrangian (17) does not possess Lorentz invariance, which makes it a qualitatively distinct theory from the versions of the SO(3) nonlinear $\sigma$ model studied in the context of classical critical phenomena. Its symmetries comprise global left rotations $R \to U_L R$ with $U_L \in SO(3)$ and global right rotations $R \to R U_R$ with $U_R \in SO(2)$ (i.e., $U_R$ commuting with $P$ and $Q$). The first of these reflects invariance under rotations in spin space, whereas the other will have consequences on the spectrum of the theory: a degeneracy of the excitation branches.

It is important to stress here that in going from the discrete Heisenberg Hamiltonian (3) to the continuum Lagrangian (17) we have assumed that smooth configurations dominate the path integral. There seems to be no distinction between integer and half-integer spins within this mapping. In particular, there is no topological term of the type arising in the collinear antiferromagnetic chain ($J' < J/4$). In fact, none could exist, since the relevant homotopy group is trivial: $\pi_2(SO(3)) = 0$. However, there are qualitative differences between integer and half-integer spins in this system. The question as to why they do not appear explicitly in the field theory will be discussed in Sec. IV.
III. SPECTRUM OF THE NONLINEAR $\sigma$ MODEL

In this section we discuss the spectrum of the model defined in Eq. (17), in particular regarding the gap to excited states and the degeneracy of the excitation branches. To this end it is preferable to rewrite the Lagrangian (17) in terms of two orthonormal vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ specifying the rotation matrix $R$. Defining $\mathbf{e}_3 = \mathbf{e}_1 \times \mathbf{e}_2$, the elements of the matrix $R$ may be expressed as $R_{ab} = (\mathbf{e}_b)_a$, and $\text{tr}(Q \partial_\tau R^{-1} \partial_\tau R) = \sum_a Q_{aa}(\partial_\tau e_a)^2$. Using the fact that

$$(\partial_\tau \mathbf{e}_3)^2 = (\partial_\tau \mathbf{e}_1)^2 + (\partial_\tau \mathbf{e}_2)^2 - 2(\mathbf{e}_1 \cdot \partial_\tau \mathbf{e}_2)^2,$$

we may finally express the Lagrangian in the following form:

$$L = \frac{1}{2g} \left\{ \frac{1}{c} \left[ (\partial_\tau \mathbf{e}_1)^2 + (\partial_\tau \mathbf{e}_2)^2 - \frac{\gamma}{c} (\mathbf{e}_1 \cdot \partial_\tau \mathbf{e}_2)^2 \right] - c \left[ (\partial_\tau \mathbf{e}_1)^2 + (\partial_\tau \mathbf{e}_2)^2 \right] \right\},$$

wherein the coupling constants $g, \gamma$ and the velocity $c$ are now

$$g = \frac{2}{\sqrt{(1 + \xi)(2\xi^2 - 2\xi + 1)}},$$
$$c = J a \sqrt{1 - \xi},$$
$$\gamma = 4\xi(1 - \xi).$$

The functional integration measure associated with the fields $\mathbf{e}_{1,2}$ must incorporate the constraints $\mathbf{e}_1^2 = \mathbf{e}_2^2 = 1, \mathbf{e}_1 \cdot \mathbf{e}_2 = 0$. This may be done by introducing three Lagrange parameters $\sigma_{11}, \sigma_{22}$, and $\sigma_{12} = \sigma_{21}$, and by adding the following constraint term to the Lagrangian:

$$L_{\text{const}} = \frac{1}{2} \sigma_{ab}(\mathbf{e}_a \cdot \mathbf{e}_b - \delta_{ab}).$$

Since this model is defined in one spatial dimension, the Mermin-Wagner-Coleman theorem applies and the global SO(3) symmetry is not broken. If we extended the model to dimensions greater than 1, a broken symmetry phase could be realized, for $g$ below some critical value. In such a phase, three Goldstone modes would appear, corresponding to the three parameters of the broken SO(3) symmetry. These three Goldstone modes would have a linear dispersion relation, two of them with speed $c$ and a third with speed $c\sqrt{1 - \gamma/2}$. The most elegant way to see this is to go back to the form (17) of the Lagrangian and to substitute, in the small oscillation approximation, $R_{ab} \approx \delta_{ab} + \varepsilon_{abc}\Omega_c$, keeping the terms of order $\Omega_c^2$ only. Since the field $\Omega_c$ is unconstrained, the dispersion relations are easily read off.

In the case of an antiferromagnet on a triangular or hexagonal lattice ($\xi = \frac{1}{3}$), the two speeds are $c$ and $c\sqrt{2}$. This may also be observed within spin-wave theory, since it is a feature of the ordered phase.

However, we are interested here in the disordered phase of the model, which we shall study within the large-$N$ approach (here $N$ is the number of components of the vectors $\mathbf{e}_a$, normally 3). In the imaginary-time formalism, the partition function of the model is

$$Z = \int [d\mathbf{e}_1][d\mathbf{e}_2][d\sigma_{ab}] \exp - \int dx d\tau \mathcal{L}_E,$$

with the Euclidean Lagrangian density

$$\mathcal{L}_E = \frac{1}{2} \left\{ \left[ (\partial_\tau \mathbf{e}_1)^2 + (\partial_\tau \mathbf{e}_2)^2 \right] - g\gamma (\mathbf{e}_1 \cdot \partial_\tau \mathbf{e}_2)^2 + \left[ (\partial_\tau \mathbf{e}_1)^2 + (\partial_\tau \mathbf{e}_2)^2 \right] \right\} + \sigma_{ab} (\mathbf{e}_a \cdot \mathbf{e}_b - \frac{1}{g} \delta_{ab}),$$

where we have rescaled $\mathbf{e}_a$ by a factor $\sqrt{g}$ in order to recover the standard normalization for the kinetic term. The characteristic speed $c$ has been set to unity in order to lighten the notation; it may be restored by dimensional analysis. We will also use a Hubbard-Stratonovich decomposition of the quartic term:

$$\exp - \int dx d\tau \frac{g\gamma}{2} (\mathbf{e}_1 \cdot \partial_\tau \mathbf{e}_2)^2$$

$$= \int [d\phi] \exp - \int dx d\tau \left\{ \frac{1}{2} \phi^2 - \sqrt{g\gamma} (\mathbf{e}_1 \cdot \partial_\tau \mathbf{e}_2) \right\}.$$

We then proceed to find the large-$N$ saddle point. In other words, we assume that the auxiliary fields $\phi$ and $\sigma_{ab}$ take a constant value, which is determined by extremizing the effective potential obtained by integrating the fields $\mathbf{e}_a$. This exercise is better done in Fourier space, in which the Euclidean action with constant auxiliary fields may be written as

$$S_E = \frac{1}{2} \int \frac{dw \; dk}{2\pi 2\pi} \mathbf{e}_a^* (\omega, k) K_{ab} \mathbf{e}_b (\omega, k) + \frac{1}{2} L^2 \left[ \phi^2 - \frac{1}{g} \sigma_{ab} \partial_\tau \delta_{ab} \right],$$

$$K (\omega, k) = \left( \frac{\omega^2 + k^2 + \sigma_{11}}{\sigma_{12} - i\omega \phi \sqrt{g\gamma}} \right) \left( \frac{\sigma_{22} - k^2 + \sigma_{11}}{\sigma_{12} - i\omega \phi \sqrt{g\gamma}} \right).$$

The effective potential is then

$$V_{\text{eff}} = \frac{1}{2} \phi^2 - \frac{1}{2g} (\sigma_{11} + \sigma_{22})$$

$$+ \frac{N}{2} \int \frac{dw \; dk}{2\pi 2\pi} \ln \det K (\omega, k),$$

where we assume the system to be limited by a box of side $L$.

In terms of the variables

$$\sigma \equiv \frac{1}{2} (\sigma_{11} + \sigma_{22}) \quad \text{and} \quad \eta^2 \equiv \frac{1}{4} (\sigma_{11} - \sigma_{22})^2 + \sigma_{12}^2,$$

the saddle-point equations are the following:
The immediate solution to these equations is $\phi = \eta = 0$ and $\sigma \neq 0$, determined by the simpler equation

$$\frac{1}{g} = \frac{N}{2} \int \frac{d\omega}{2\pi \omega} \frac{1}{\omega^2 + k^2 + \sigma}.$$  

(31)

It can be shown explicitly that the solution $\phi = \eta = 0$ is the only acceptable one in this case. Equation (31) coincides with the saddle-point equation for the O(3)/O(2) nonlinear $\sigma$ model, whose solution is

$$\sigma = \sigma_0 \equiv \Lambda^2 \exp\left(-\frac{8\pi}{3g}\right),$$  

(32)

wherein $\Lambda$ is a momentum cutoff. The fields $\sigma_{11}$ and $\sigma_{22}$ must therefore be shifted by the constant $\sigma_0$ in order to fluctuate about zero. Then $\sigma_0$ multiplies $\frac{1}{2} e_1^2$ and $\frac{1}{2} e_2^2$ in the large-$N$ effective action; thus, it has the interpretation of a quantum fluctuation-induced mass squared for the fields $e_2$. The excitations of these fields are then triplets with energy gap $\Delta = \Lambda \exp\left(-4\pi/3g\right)$. After restoring the characteristic speed $c$, and the dependence on $\xi$, this becomes

$$\Delta = (\Lambda a) J s \frac{1 + \xi}{\xi} \left(\frac{1 - \xi^2}{(2\xi^2 - 2\xi + 1)}\right)^{\frac{1}{2}} x \exp\left(-\frac{1}{2\xi}\right).$$  

(33)

Of course, this result neglects $1/N$ corrections. First $1/N$ corrections to the mass gap of the O(3)/O(2) model have been computed and bring logarithmic corrections to Eq. (32), which do not qualitatively alter the picture. According to Eq. (33), the gap increases and becomes eventually proportional to $J'$, as $\xi$ goes from 1 ($J' = \frac{1}{2} J$) to 0 ($J' \rightarrow \infty$). The conclusion that the gap goes to zero as $\xi \rightarrow 1$ is also arrived at if the point $J' = \frac{1}{2} J$ is approached from below, using the semiclassical mapping to the O(3)/O(2) nonlinear $\sigma$ model, since in that case also the characteristic velocity $v$ goes to zero as $J' \rightarrow \frac{1}{4} J$.  

$$v = 2 Jas \sqrt{1 - \frac{4J'}{J}}.$$  

(34)

However, this conclusion about the vanishing of the gap at $J' = \frac{1}{4} J$ (or at any value of $J'$) is probably erroneous, in light of exact diagonalizations for finite chains. We will come back to this point in the next section.

The main feature of the excitations of this model is the degeneracy of the triplets. This ultimately comes from the SO(2) symmetry existing between the vectors $e_1$ and $e_2$, which may be mixed with each other without affecting the action. It is then not surprising if this degeneracy survives the large-$N$ approximation.

Indeed, $1/N$ corrections to the dispersion of the excitations can in principle be calculated, like they are in the O(3)/O(2) $\sigma$ model (see, for instance, Polyakov’s text). The quantity of interest is then the self-energy of the fields $e_2$. In general, this is a matrix $\Sigma_{ab}(\omega, k)$, which may be calculated diagrammatically with the help of the vertices shown in Fig. 2 and of the propagators for the auxiliary fields $a_{ab}$ and $\phi$. The latter scale as $1/N$ since they are inverse polarization operators, and the order in $1/N$ is simply determined by the number of auxiliary field internal lines. However, the propagators for $a_{11}$ and $a_{22}$ are identical, since the large-$N$ propagators of $e_1$ and $e_2$ are the same. Moreover, the structure of the vertices of Fig. 2 makes it impossible for a nondiagonal self-energy $\Sigma_{12}$ to arise: Even though the auxiliary fields $a_{12}$ and $\phi$ may change an $e_1$ quantum into an $e_2$ quantum, the number of such vertices must be even, without tadpoles. The net result is that no self-energy diagram exists in which an entering $e_1$ line is turned into an exiting $e_2$ line, and consequently $\Sigma_{12} = 0$. The $1/N$ contributions to the $\Sigma_{11}$ are shown diagrammatically on Fig. 3. At all orders in $1/N$ the two self-energies $\Sigma_{11}$ and $\Sigma_{22}$ are identical and therefore the degeneracy of the excitations branches seems an exact feature of the model.

IV. DISCUSSION

In Sec. II we argued that the frustrated AF spin chain may be described, in the continuum limit, by the SO(3) nonlinear $\sigma$ model defined by the Lagrangian (17). In Sec. III, we argued that the main feature of the spectrum of this continuum model is a doubly degenerate triplet of spin-1 excitations, separated from the singlet ground

FIG. 2. Vertices used in the $1/N$ expansion of the model (27).
state by a gap. However, this conclusion is incompatible with what is known of the spectrum of the frustrated spin-\(\frac{1}{2}\) chain. The Lieb-Schultz-Mattis (LSM) theorem\(^{18}\) states that a spin-\(\frac{1}{2}\) chain has either no gap or degenerate ground states (corresponding to spontaneously broken parity). More recently, it has been shown\(^{19}\) that this theorem applies to half-integer spin chains in general. In the special case \(J' = J/2\) the exact ground state of the spin-\(\frac{1}{2}\) chain obtained by Majumdar and Gosh\(^{6}\) is twofold degenerate. This is compatible with the LSM theorem, but in contradiction with the field theory. Thus, the latter does not correctly describe frustrated half-integer spin chains.

Before throwing the SO(3) model away, one should see if it describes the long-wavelength behavior of integer spin chains. Exact results for the spin-1 chain are lacking and thus we are reduced to numerical study of finite systems. Quantum Monte Carlo studies of frustrated spin systems are quite difficult because of a sign problem; therefore we limited ourselves to numerical diagonalizations of small chains (up to 14 sites). We used various methods, of which the most practical turned out to be a variant of the Lanczos method\(^{20}\) applied to subspaces of fixed momentum. Diagonalizations of spin-\(\frac{1}{2}\) chains with up to 22 sites have also been performed, for the sake of comparison. It turns out that the spectra of spin-1 and spin-\(\frac{1}{2}\) chains of small lengths are qualitatively different. The ground state of the spin-1 chains is nondegenerate, with a gap to a doubly degenerate triplet of spin-1 states, exactly as in the field theory. Excitation spectra for \(J' = J/2\) and various chain lengths are shown in Fig. 4, whereas spectra for 14 spins and various values of \(J'/J\) are shown in Fig. 5. The dispersion relation is symmetric with respect to parity \((k \rightarrow -k)\) and the minimum of the spin-1 branch occurs at a wave number \(k_0\) smaller than \(\pi\) (in units of \(1/\alpha\)). Consequently, this minimum also occurs at \(-k_0\), which is distinct from \(k_0\) except at the ferromagnetic \((k = 0)\) and antiferromagnetic \((k = \pi)\) points. The existence of these minima away from the parity-invariant points should not surprise us. If it were not for the quantum fluctuation disordering the system, there would be massless Goldstone branches around the ordering wave vectors \(k_0 = \alpha\) and \(-k_0\) [\(\alpha\) is given by Eq. (4)]. The effect of quantum fluctuations is to produce a singlet ground state and to raise the minima of the Goldstone branches. We expect that the positions of these minima will be approximately the same as the classical ordering wave vectors \(k_0\) and \(-k_0\), although we have no way to prove that they coincide exactly with these values. The SO(3) field theory effectively describes low-energy excitations about the minima of these excitation branches, and the degeneracy is essentially linked to the fact that the classical ordering wave vectors \(k_0\)

and \(-k_0\) are inequivalent. This feature of the excitation spectrum supports the view that the SO(3) field theory describes the long-wavelength behavior of the frustrated spin-1 chain.

It should be pointed out that, in a chain of length \(N\), there is critical value \(\xi_c(N)\) of the ratio \(J'/4J\), above which the minimum in the triplet dispersion relation occurs at \(k = \pi\). This critical value depends on the length of the chain. Figure 6 shows the evolution of \(\xi_c\) for small sizes,
as well as the value of the mass gap $\Delta$. If one trusts the heuristic mapping of Sec. II, $\xi_c$ should be equal to 1 when $N \to \infty$. For finite chains it is closer to 0.6 (i.e., $J'/J \sim 0.4$). A similar conclusion is reached in Ref. 7. This means that the semiclassical mapping of Sec. II must receive important quantum corrections: The parameters $\nu$ and $g$ obtained from this naive mapping must be renormalized. This raises another question: The characteristic velocity $v$ obtained semiclassically vanishes at the transition point $\xi_c$, thus leading to the hasty conclusion that the gap vanishes at this point. However, such an inflexion of the gap around $\xi_c$ is not observed in exact diagonalizations, either in this work or in Ref. 7. Instead, what probably happens is that the effective mass $m^* = \left[ \frac{\partial^2 \epsilon(k)}{\partial k^2} \right]^{-1}$ diverges at the transition, while the excitation gap $\Delta$ stays finite. The Lorentz-invariant O(3)/O(2) $\sigma$ model predicts $\Delta^2 = m^* v^2$, but the case $v \to 0$, $m^* \to \infty$ is surely pathological and difficult to interpret. Our trust in the nonlinear field theories should be limited to situations in which the dispersion curve is clearly parabolic around the ordering point(s).

The question remains as to why this semiclassical treatment fails in the half-integer spin case. In other words, where in the argument of Sec. II should the distinction between integer and half-integer spin come into play? The answer may lie in our neglect of configurations with discontinuities. This has already been pointed out in Ref. 4 in relation with the kinetic term. An easier way to see this is to consider the limit $J' \gg J$. In that limit one may reconsider the problem and view the system as a pair of interwoven, antiferromagnetic chains with a small interchain interaction $J$. Each chain could be semiclassically described by the usual O(3)/O(2) nonlinear $\sigma$ model, with the Lagrangian density (1), plus a topological term $\mathcal{L}_{\top}$ expressed as

$$\mathcal{L}_{\top} = -\frac{g}{2} \mathbf{e} \cdot (\partial_t \mathbf{e} \times \partial_2 \mathbf{e}) \ .$$

(35)

Since the effective lattice spacing for each chain is now $\tilde{a} = 2a$, the characteristic velocity would be $c = 4J'as$, while the coupling constant is still $g = 2/s$. One checks that this agrees perfectly with the $\xi \to 0$ limit of Eq. (22). Thus, as $\xi = J/4J'$ decreases, the two unit vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ of the SO(3) model become the fields of two weakly coupled O(3)/O(2) $\sigma$ models, with the correct values of $c$ and $g$.

The interaction $\mathcal{L}_{\text{int}}$ between the two chains may be easily expressed in terms of $\mathbf{e}_1$ and $\mathbf{e}_2$. Indeed, recall that in taking the continuum limit of a single AF chain, one uses the decomposition $S_i = s((-1)^i \mathbf{e} + \tilde{a} \hat{l})$, where $\hat{l}$ is the local magnetization and $\tilde{a} = 2a$ is the effective lattice spacing for each chain. Neglecting derivatives, the interaction Lagrangian may be written as

$$\mathcal{L}_{\text{int}} = -2J s^2 \tilde{a} l_1 \cdot l_2 \ .$$

(36)

The elimination of $l_1$ and $l_2$ is done by substituting the equation of motion \(^{11}\)

$$l_\alpha = -\frac{1}{4J s^2} (\mathbf{e}_\alpha \times \partial_t \mathbf{e}_\alpha) \ .$$

(37)

The interaction Lagrangian then becomes

$$\mathcal{L}_{\text{int}} = -\frac{1}{16a J} \frac{J}{J'} (\mathbf{e}_1 \times \partial_t \mathbf{e}_1) \cdot (\mathbf{e}_2 \times \partial_t \mathbf{e}_2) \ .$$

(38)

$$\mathcal{L}_{\text{int}} = -\frac{1}{16a J} \xi^2 \left\{ \mathbf{e}_1 \cdot \mathbf{e}_2 \partial_t \mathbf{e}_1 \cdot \partial_t \mathbf{e}_2 - \mathbf{e}_1 \cdot \partial_t \mathbf{e}_2) (\mathbf{e}_2 \cdot \partial_t \mathbf{e}_1) \right\} \ .$$

(39)

If we assume that the two vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ are identically orthogonal, as the classical ground state suggests if $\xi$ is small, then the above interaction exactly agrees with Eq. (21) and the $\xi \to 0$ limit of $\gamma$ as given in Eq. (22). Moreover, the topological terms $S_{\text{top}}[\mathbf{e}_1]$ and $S_{\text{top}}[\mathbf{e}_2]$ cancel each other if $\mathbf{e}_1$ is identically orthogonal to $\mathbf{e}_2$. This is particularly easy to understand if the configuration $\mathbf{e}_1$ belongs to the homotopy class of the identity, since the orthogonality constraint then effectively makes $\mathbf{e}_2$ a mapping from the sphere $S_2$ to the circle $S_1$ and $\pi_2(S_1) = 0$. In general, the two topological terms cancel simply because of the fact that two orthogonal unit vectors specify a rotation and $\pi_2(SO(3)) = 0$. Thus, if we assume that $\mathbf{e}_1 \perp \mathbf{e}_2$ in the small $\xi$ limit, the Lagrangian (21) is recovered with exactly the same parameters, since the topological terms are absent.

However, the orthogonality $\mathbf{e}_1 \perp \mathbf{e}_2$ is not strict, but only favored energetically. A local deviation from this orthogonality gives back their full importance to the topological terms and causes a distinction between integer and half-integer spins. Such a distinction does not occur in the SO(3) formulation of the problem since the orthogonality is then "built in." In that formulation, a local deviation from orthogonality corresponds to a discontinuity in the order parameter, which was not allowed from the start.

Finally, let us point out that the above remarks concerning parity-breaking ordering wave vectors in frustrated antiferromagnets and their consequences on the excitation spectrum may apply to other systems, such as the nearest-neighbor Heisenberg antiferromagnet on a triangular lattice. In this case it is believed that the
ground state has long-range order. However, it is conceivable that the introduction of vacancies destroys this order without affecting the applicability of the SO(3) theory: The effect of the vacancies would then be to increase the value of the effective coupling constant $g$ beyond the critical value $g_c$. A priori, it is not clear if the SO(3) field theory describes the long-wavelength behavior of antiferromagnets on the \textit{kagomé} lattice or on the seesaw chain.\textsuperscript{21} A semiclassical study of these systems may be interesting.

\section*{Acknowledgments}

The authors thank L. Chen, A. Chubukov, A.-M. S. Tremblay, and G. Zumbach for stimulating discussions. Financial support from the Natural Sciences and Engineering Research Council of Canada (NSERC) and \textit{le} Fonds pour \textit{la} Formation de Chercheurs et \textit{et} \textit{l'Aide à la Recherche du Gouvernement du Québec} (FCAR) is gratefully acknowledged.

\begin{thebibliography}{19}
\bibitem{17} A. M. Polyakov, \textit{Gauge Fields and Strings} (Harwood, New York, 1987).
\end{thebibliography}