Effect of small interchain coupling on one-dimensional antiferromagnetic quantum Heisenberg spin systems: The integer-spin case

M. Azzouz* and B. Douçot
Centre National de la Recherche Scientifique, Centre de Recherches sur les Très Basses Températures, Boîte Postale 166, 38042 Grenoble CEDEX 9, France
(Received 27 July 1992)

A two-dimensional array of weakly coupled antiferromagnetic spin chains is investigated using the Schwinger-boson technique. This method is known to give a good description of integer spins already at the mean-field level. We find that a finite coupling is necessary to introduce long-range antiferromagnetic order, consistently with the presence of a gap for a single chain. The energy gap and spin-spin correlations are calculated. These calculations correspond to the behavior of a nonlinear σ model without the one-dimensional topological term.

I. INTRODUCTION

The discovery of high-temperature superconductivity has stimulated much activity in the field of strongly correlated and low-dimensional systems. In this paper, we study the effect of a weak interchain coupling on a quantum antiferromagnetic two-dimensional array of spin chains. For an isolated chain, strong quantum fluctuations destroy long-range order even at zero temperature. However, for an isotropic two-dimensional unfrustrated lattice, it has been rigorously proved that there is a long-range Néel order for $S \geq 1$,[1] and this is widely believed to be the case for $S=\frac{1}{2}$ also. The question we address is whether this ordering occurs in the presence of any infinitesimal transverse coupling or not. Actually, for an XY model, the 1D chain is gapless, with power-law spin-spin correlations. As a result, the staggered spin susceptibility is infinite and we expect that long-range order arises immediately at any finite coupling. The situation is different in the case of the Heisenberg model. Indeed, it was first pointed out by Haldane that isolated integer spin chains with nearest-neighbor coupling have a finite correlation length and an energy gap, whereas half integer spins remain massless.[2] From this picture, one would expect that a finite transverse coupling is required to generate long-range order in the integer spin case. For half integer spins, the situation is much less obvious, since the absence of a gap is due to a topological term in the long wavelength effective action. This topological term has a dramatic influence in the pure one-dimensional case, but is expected to have much less of an effect in two dimensions.[3] We then have a competition between the tendency towards ordering and the loss of strict one dimensionality which may suppress the action of the topological term.

In this paper, we shall use the mean-field Schwinger-boson method. It has been shown that this formalism provides a very good description of singlet disordered states such as in the two-dimensional system at finite temperature, and the one-dimensional chain at $T=0$.[4,5] The results obtained there are quite similar to the behavior of the nonlinear σ model which is the effective long-wavelength action in the absence of a topological term. In this respect, our treatment is mostly relevant to the integer spin case. Other methods should be used to treat properly half integer spins. We hope to address this question in the near future.

This work has also been motivated by recent ideas about the normal state of high-T_c materials.[6,7] These authors suggest that a Luttinger liquid may exist in more than one dimension. This statement has to be contrasted with weak-coupling renormalization-group arguments, which claim that transverse coupling between chains is always relevant and destroys the Luttinger liquid.[8] Weakly coupled spin chains may provide some insight in understanding these issues better. However, as already stressed, the most interesting situation, namely, for half integer spin, is not accessible by our method.

In the first part, the Schwinger-boson formalism is used to obtain mean-field equations in the presence of anisotropic couplings. The behavior of the gap is then studied in the second part. We show that a finite coupling is necessary to stabilize long-range Néel order and calculate the phase boundary as a function of spin S. Furthermore, spin-spin correlation functions are also calculated. The conclusion is devoted to a comparison with experimental observations on spin 1 quasi-unidimensional spin chains. We also make a few remarks on the half-integer-spin problem.

II. DERIVATION OF MEAN-FIELD EQUATIONS

A. Schwinger bosons

The SU(2) antiferromagnetic model on the anisotropic square lattice is given by the Hamiltonian

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_\perp \sum_{\langle l,m \rangle} \mathbf{S}_l \cdot \mathbf{S}_m \ , \tag{1}$$

where the sums $\langle i,j \rangle$ and $\langle l,m \rangle$ are defined for the first nearest neighbors along the x and y directions, respectively. J is the exchange coupling on the x axis and $J_\perp$ is

the one on the y axis. Weakly coupled spin chains correspond to the limit $J_\perp/J \ll 1$. Before extending the model to SU(N) symmetry, let us review the Schwinger-boson formalism in the case of $N=2$. In this representation, the spin operators are written as follows[4]:

$$S^+ = a^\dagger b, \quad S^- = ab^\dagger, \quad S^z = \tfrac{1}{2}(a^\dagger a - b^\dagger b) ,$$

with the holonomic constraint $2S = n_a + n_b$, where $n_a = a^\dagger a$ and $n_b = b^\dagger b$ are the number of the a and b bosons, respectively. The commutation relations of the spin components are satisfied. If we assume that the lattice is bipartite (Fig. 1), and so there is no frustration, then on one sublattice we perform the unitary transformation $a \to -b$ and $b \to a$, i.e., S^+ is transformed in $-ab^\dagger$.

The generalized SU(N) Hamiltonian is

$$H = -\frac{J}{N} \sum_{\substack{\langle i,j \rangle \\ \alpha,\beta}} S^\alpha_\beta(i) \tilde{S}^\beta_\alpha(j) - \frac{J_\perp}{N} \sum_{\substack{\langle l,m \rangle \\ \alpha,\beta}} S^\alpha_\beta(l) \tilde{S}^\beta_\alpha(m) , \qquad (2)$$

where $S^\alpha_\beta(i)$ [$\tilde{S}^\alpha_\beta(j)$] is the generalized spin on sublattice A (on sublattice B) defined by

$$S^\alpha_\beta(i) = b^\dagger_{\alpha i} b_{\beta i} \quad [\tilde{S}^\alpha_\beta(j) = -b^\dagger_{\beta j} b_{\alpha j}] .$$

The constraint becomes

$$\sum_{\alpha=1}^{N} S^\alpha_\alpha(i) = NS \quad \left[\sum_{\alpha=1}^{N} \tilde{S}^\alpha_\alpha(j) = NS \right] .$$

Equation (2) may be expressed in a set of new variables A_{ij}

$$A_{ij} = \sum_{\alpha=1}^{N} b_{\alpha i} b_{\alpha j}$$

and this reads

$$H = -\frac{J}{N} \sum_{\langle i,j \rangle} A^+_{ij} A_{ij} - \frac{J_\perp}{N} \sum_{\langle l,m \rangle} A^+_{lm} A_{lm} . \qquad (3)$$

The resulting Hamiltonian is not invariant under a global SU(N) transformation U, but under staggered transformations, namely, U on A and U^+ on B, respectively.

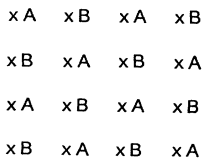

FIG. 1. Illustration of the sublattice definition on the square lattice.

B. Path-integral formulation

Once the Hamiltonian is written in the bosonic operators $b_{\alpha i}$ the partition function can be given by the coherent state functional integral[4]:

$$Z = \int D(b,\bar{b},\lambda) \exp[-J(b,\bar{b};\lambda)]$$

where the action $J(b,\bar{b};\lambda)$ is

$$J(b,\bar{b};\lambda) = \int_0^\beta d\tau \left[\sum_{i,\alpha} \bar{b}_{\alpha i} \frac{\partial}{\partial\tau} b_{\alpha i} - \frac{J}{N} \sum_{\langle i,j \rangle} A^-_{ij} A_{ij} - \frac{J_\perp}{N} \sum_{\langle l,m \rangle} A^-_{lm} A_{lm} + \sum_{i,\alpha} \lambda_i (\bar{b}_{\alpha i} b_{\alpha i} - S) \right] , \qquad (4)$$

where $b_{\alpha i}$ is a c number, $\bar{b}_{\alpha i}(\tau)$ is its complex conjugate, and λ_i is a Lagrange factor which imposes the occupation constraint. Using two Hubbard-Stratonovich fields for every bond: Q_{ij} along x axis and P_{lm} along y axis, the biquadratic interaction terms may be decoupled, resulting in

$$Z = \int D(b,\bar{b};Q,\bar{Q},P,\bar{P};\lambda) e^{-I}$$

with now:

$$I = \int_0^\beta d\tau \left[\sum_{i,\alpha} \bar{b}_{\alpha i} \frac{\partial}{\partial\tau} b_{\alpha i} + \frac{N}{J} \sum_{\langle i,j \rangle} \bar{Q}_{ij} Q_{ij} + \sum_{\langle i,j \rangle} (\bar{Q}_{ij} A_{ij} + Q_{ij} \bar{A}_{ij}) + \frac{N}{J_\perp} \sum_{\langle l,m \rangle} \bar{P}_{lm} P_{lm} + \sum_{\langle l,m \rangle} (\bar{P}_{lm} A_{lm} + P_{lm} \bar{A}_{lm}) + \sum_{i,\alpha} \lambda_i (\bar{b}_{\alpha i} b_{\alpha i} - S) \right] . \qquad (5)$$

Q_{ij} and P_{lm} are interpreted as effective hopping terms depending respectively on the bonds $\langle i,j \rangle$ and $\langle l,m \rangle$, and the time τ. $Q_{ij} = |Q_{ij}| e^{i\phi_{ij}}$, $P_{lm} = |P_{lm}| e^{i\psi_{lm}}$, and λ_i is a pure complex function of the site position and τ. In one dimension ($P_{lm} = 0$), the phase ϕ_{ij} of Q_{ij} can be eliminated by a time-dependent Read-Newns gauge transformation[11] which replaces the integration over Q_{ij} by an integration over only the magnitude $|Q_{ij}|$. The phase ϕ_{ij} then plays no role in the difference between integer and half-integer spin chains. Now, when the chains are weakly coupled, the phases ϕ_{ij} and ψ_{lm} cannot be eliminated by a gauge transformation, but we will suppose that the relevant saddle points correspond to a fluxless configuration. This choice is motivated by the success of such a mean-field approach for the isotropic two-dimensional system.[4] Thus, we search for solutions where Q_{ij} and P_{lm} are equal to their magnitudes, respectively. λ_i is also replaced by its magnitude at the mean-field level.[12]

The mean-field equations are obtained at the saddle point which is given by minimizing the action with respect to $Q_{ij}(\tau)$, $P_{lm}(\tau)$, and $\lambda_i(\tau)$:

$$\frac{\partial I}{\partial Q_{ij}(\tau)}=\frac{\partial I}{\partial P_{lm}(\tau)}=\frac{\partial I}{\partial \lambda_i(\tau)}=0 \ . \tag{6}$$

We shall restrict ourselves to uniform and time-independent saddle points. This means that we take $|Q_{ij}|=Q$, $|P_{ij}|=P$, and $|\lambda_i|=\lambda$, all of them time and space independent. After easy calculations, we get the following mean-field Hamiltonian k space:

$$H^{\mathrm{MF}}=N_S\frac{N}{J}Q^2+N_S\frac{N}{J_\perp}P^2-NN_SS\lambda$$
$$+\frac{1}{2}\sum_{\mathbf{k},\alpha}[\lambda(b^\dagger_{\mathbf{k},\alpha}b_{\mathbf{k},\alpha}+b^\dagger_{-\mathbf{k},\alpha}b_{-\mathbf{k},\alpha})+(2Q\cos k_x+2P\cos k_y)(b_{k,\alpha}b_{-k,\alpha}+b^\dagger_{k,\alpha}b^\dagger_{-k,\alpha})] \ ,$$

with N_s is the total number of sites. H^{MF} is diagonalized by a Bogoliubov transformation. The mean-field free energy is obtained after integration over the bosonic variables

$$\frac{F^{\mathrm{MF}}}{N_sN}=\frac{Q^2}{J}+\frac{P^2}{J_\perp}-\frac{\lambda}{2}(2S+1)+\frac{1}{\beta}\times\int\frac{d\mathbf{k}}{(2\pi)^2}\ln\left[2\sinh\left[\frac{\beta\omega_k}{2}\right]\right] , \tag{8}$$

where

$$\omega_k=[\lambda^2-4(Q\cos k_x+P\cos k_y)^2]^{1/2} \tag{9}$$

is the dispersion relation at the mean-field level. The mean-field equations, derived from the saddle-point condition, are as follows:

$$\frac{Q}{J}=\int\frac{d^2k}{(2\pi)^2}\coth\left[\frac{\beta\omega_k}{2}\right]\times\omega_k^{-1}\cos k_x(Q\cos k_x+P\cos k_y) \ , \tag{10}$$

$$\frac{P}{J_\perp}=\int\frac{d^2k}{(2\pi)^2}\coth\left[\frac{\beta\omega_k}{2}\right]\times\omega_k^{-1}\cos k_y(Q\cos k_x+P\cos k_y) \ , \tag{11}$$

$$\frac{2S+1}{\lambda}=\int\frac{d^2k}{(2\pi)^2}\coth\left[\frac{\beta\omega_k}{2}\right]\omega_k^{-1} \ . \tag{12}$$

The integration $\int d^2k/(2\pi)^2$ is taken over the first Brillouin zone. The above three equations constitute the mean-field solution to this problem. In the following, we will define the reduced variables:

$$\tilde{Q}=\frac{Q}{\lambda} \quad \text{and} \quad \tilde{P}=\frac{P}{\lambda} \ .$$

III. ANALYSIS OF MEAN-FIELD EQUATIONS AT $T=0$

The energy spectrum is given by

$$\omega_k=[\lambda^2-4(Q\cos k_x+P\cos k_y)^2]^{1/2} \ ,$$

where Q, P, and λ are functions of J, $J_\perp$, and the spin S [Eqs. (10)–(12)]. It exhibits an energy gap

$$\Delta=[\lambda^2-4(Q+P)^2]^{1/2} \ .$$

We shall show below that Δ is a decreasing function of $J_\perp/J$ and goes continuously to zero at a critical value $(J_\perp/J)_c$ which depends on the value of the spin S. This behavior of Δ indicates a second-order transition from a one-dimensional disordered phase to a two-dimensional phase with long-range Néel order. The presence of a finite gap Δ in the one-dimensional region suggests that the method does not allow us to study half integer spins, and that only the case of integer spins can be treated here.[9]

A. Calculation of the critical value of $J_\perp/J$ at the transition

The divergence of the correlation length ξ as the energy gap Δ vanishes ($\xi\sim 1/\Delta$) is a consequence of the second-order transition. The condition $\Delta=0$ yields:

$$\lambda^2-4(Q+P)^2=0 \ . \tag{13}$$

In connection with Eq. (12), the above equation [Eq. (13)] gives for large S (see Appendix A)

$$P/Q\approx e^{-\pi(2S)} \ . \tag{14}$$

In the same spirit as in Appendix A, Q/J and $P/J_\perp$ are found to be

$$\frac{Q}{J}\approx\frac{1}{\pi}\ln\left[\frac{\tilde{Q}}{\tilde{P}}\right] , \tag{15}$$

$$\frac{P}{J_\perp}\approx 2\left[\frac{1}{\pi}+\frac{1}{\sqrt{2}}\right]\sqrt{\tilde{Q}} \ . \tag{16}$$

From Eqs. (14)–(16) the critical value $(J_\perp/J)_c$, where the system has this second-order transition from the one-dimensional to the two-dimensional regime, is calculated for large S. We have:

$$(J_\perp/J)_c\sim Se^{-2\pi s} \ . \tag{17}$$

It becomes obvious that for large spin S, a finite value of the transverse coupling $J_\perp$ is needed to get the antiferromagnetic long-range order, in agreement with Ref. 10. Spin-wave theory gives a similar asymptotic behavior for $(J_\perp/J)_c$. We found $(J_\perp/J)_c\sim e^{-\pi(2S)}$. In fact, in spin-wave theory, $(J_\perp/J)_c$ is calculated imposing the condition that the correction to the Néel magnetization is such that $\langle S^z\rangle=0$. This condition leads to the following equation[22]:

$$\langle S^z\rangle=\frac{1}{2}\left[2S+1-\int\frac{d^2k}{(2\pi)^2}\frac{J_\perp+J}{[(J_\perp+J)^2-(J\cos k_x+J_\perp\cos k_y)^2]^{1/2}}\right]=0\ . \tag{18}$$

We know that if $J_\perp=0$, the integral in Eq. (18) is equal to $-\infty$. This implies that the standard spin-wave theory is uncontrolled in the case of one-dimensional systems. But the correction introduced, when $J_\perp$ is finite, behaves as $\ln(J_\perp/J)$. The condition $\langle S^z\rangle=0$ means that the lowest-order in spin-wave theory becomes self-consistent, and this appears to not be equivalent to the onset of a phase with long-range order where $\langle S^z\rangle$ is not equal to zero. However, the precise reason for the discrepancy between the result of Eq. (17) and the result of spin-wave theory, for $(J_\perp/J)_c$, is not well understood yet.

When $J_\perp/J$ is larger than the critical value the energy gap remains equal to zero. As noted by Arovas and Auerbach,[4] the mean-field equations do not have solutions for $S\geq 0.2$ in the isotropic case, $J_\perp=J$. Above $(J_\perp/J)_c$, a Bose condensation at $T=0$ must exist in the ordered phase because a nonsymmetry breaking mean-field solution does not exist. This Bose condensation is equivalent to a two-dimensional Néel ordered phase.

The result of Eq. (17) can be written in the following asymptotic form for the large spin S:

$$(J_\perp/J)_c\sim\xi_{1D}^{-2}\ , \tag{19}$$

where $\xi_{1D}\sim e^{\pi s}$ is the one-dimensional antiferromagnetic correlation length. With this analysis we get the condition satisfied by the couplings J and $J_\perp$ ($J_\perp\xi_{1D}^2\sim J$) in order to have the transition from a disordered to an ordered antiferromagnetic phase. Equation (19) can be derived if we say that the transverse coupling times the one-dimensional correlation length must be of the order of the gap. But, following a naive argument saying that the critical transverse coupling should be of the order of the one-dimensional gap $\Delta\sim e^{-\pi s}$ gives

$$(J_\perp/J)_c\sim\xi_{1D}^{-1}\ , \tag{20}$$

where the exponent is minus unity instead of 2 as in Eq. (19). Note that as the gap is equal to zero in the case of spin $\frac{1}{2}$, the above arguments would give a critical transverse coupling $J_\perp=0$ because $\xi_{1D}=\infty$. This question is still unsettled.

B. Energy gap Δ

Analytical expressions for the energy gap will be given both in the vicinities of the one-dimensional limit and the transition. The one-dimensional limit is defined by $J_\perp/J\ll(J_\perp/J)_c$. An approximate evaluation of the energy gap Δ in the large spin limit gives

$$\Delta\sim Se^{-\pi(S)}\left[1-\frac{\pi^4}{384}\left[\frac{e^{\pi(2s)}}{2S}\right]^2\left[\frac{J_\perp}{J}\right]^2\right]J \tag{21}$$

in the one-dimensional limit and

$$\Delta\sim J\left[\left[\frac{J_\perp}{J}\right]_c-\frac{J_\perp}{J}\right]^{1/2} \tag{22}$$

in the vicinity of the transition.

The asymptotic behavior of the gap, as a function of the spin S in the case of $J_\perp=0$, $\Delta\sim Jse^{-\pi s}$, is in agreement with the result of Arovas and Auerbach.[4] A correction term quadratic in $J_\perp/J$ rather than linear in $J_\perp/J$ is obtained for Δ in Eq. (21).

C. Phase diagram

The problem we are studying depends on two parameters at zero temperature: the spin S and the ratio $J_\perp/J$. For fixed S, the phase space shown in Fig. 2 is one-dimensional. The critical value $(J_\perp/J)_c$ separates two regions, the first one (A), which is characterized by

$$J_\perp/J<(J_\perp/J)_c\ ,$$

is a disordered phase while the second one (B), which is given

$$(J_\perp/J)_c<J_\perp/J\ ,$$

does have antiferromagnetic long-range Néel order.

Now, if the spin is allowed to take any value, Eq. (17) will allow us to draw the $[1/S,(J_\perp/J)_c]$ phase diagram (Fig. 3), for large spin value S. On the same figure we draw the boundary which we get from the spin-wave theory analysis. Note that the discrepancy between these results is not very important. No transverse coupling $J_\perp$ is required to obtain long-range order in the classical limit $S=\infty$. But for finite S, quantum fluctuations destroy the antiferromagnetic order so that $(J_\perp/J)_c$ is finite but exponentially small.

D. Asymptotic spin-spin correlation functions

We are interested in calculating the asymptotic behavior of the correlation functions as the distance $\|\mathbf{R}\|$ goes to infinity. These functions have the form[4]

$$\langle\mathbf{S}_0\cdot\mathbf{S}_\mathbf{R}\rangle=\tfrac{3}{2}|f(\mathbf{R})|^2-\tfrac{3}{2}|g(\mathbf{R})|^2\ . \tag{23}$$

We restrict ourselves to the calculation of the antiferromagnetic correlation functions in the x and y directions and take, respectively, $\mathbf{R}=(R_x,0)$ or $\mathbf{R}=(0,R_y)$. The

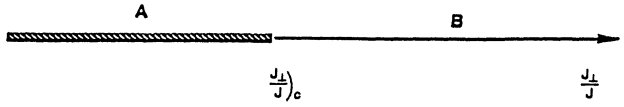

FIG. 2. $J_\perp/J$ phase diagram for a fixed spin value S.

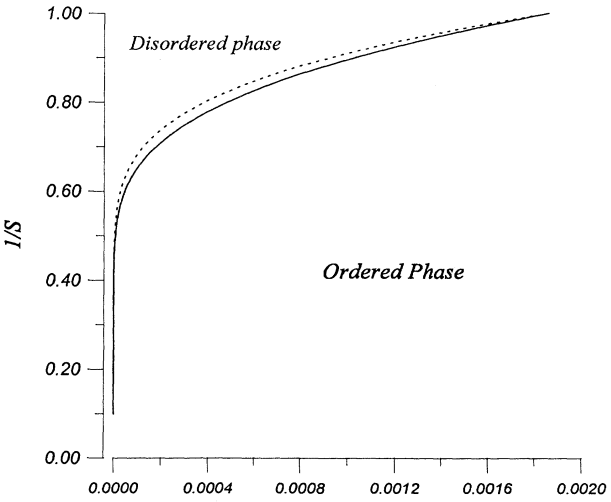

FIG. 3. $[1/S, (J_\perp/J)_c]$ phase diagram. The solid line is the result of the Schwinger-boson analysis and the dashed one is the result of an approximate evaluation of Eq. (18) obtained from the spin-wave analysis. These lines separate the antiferromagnetically ordered phase from the disordered one.

quantities $f(\mathbf{R})$ and $g(\mathbf{R})$ are given by

$$f(\mathbf{R})=\frac{1}{2}\int \frac{d^2k}{(2\pi)^2}e^{i\mathbf{kR}}\frac{1}{[1-4(\tilde{Q}\cos k_x+\tilde{P}\cos k_y)^2]^{1/2}}\ , \tag{24}$$

$$g(\mathbf{R})=\frac{1}{2}\int \frac{d^2k}{(2\pi)^2}e^{i\mathbf{kR}}\frac{\tilde{Q}\cos k_x+\tilde{P}\cos k_y}{[1-4(\tilde{Q}\cos k_x+\tilde{P}\cos k_y)^2]^{1/2}}\ . \tag{25}$$

We can show that whenever R_x or R_y belongs to the odd sublattice $f(\mathbf{R})$ vanishes, and that whenever R_x or R_y is on the even sublattice $g(\mathbf{R})$ vanishes (recall that the lattice is bipartite).

The asymptotic expressions of $\langle \mathbf{S}_0\mathbf{S}_R\rangle$ in the vicinities of the one-dimensional limit and of the critical coupling are calculated for both the x and y directions. We can refer to Appendix B for the expressions of $\tilde{P}$ and $\tilde{Q}$ and the definition of m which appears below. For correlations along the x axis, we get the following: in the one-dimensional limit, $R_x \equiv R$, and m is finite so that

$$\langle \mathbf{S}_0\mathbf{S}_R\rangle \sim -\frac{\tilde{Q}+\tilde{P}}{\tilde{Q}}\frac{3\pi}{4}\left[\frac{1}{2\pi}-\frac{\pi}{12}\frac{\tilde{P}}{\tilde{Q}}\frac{R}{m}\right]^2\frac{e^{-2mR}}{mR}\ ; \tag{26}$$

and in the vicinity of the transition ($mR \gg 1$), we have

$$\langle \mathbf{S}_0\mathbf{S}_R\rangle \sim -\frac{3}{32\pi^3}\frac{\tilde{Q}+\tilde{P}}{\tilde{Q}}\left[1+\frac{1}{mR}\right]^2\frac{m}{R}e^{-2mR}\ . \tag{27}$$

Along the y axis, the correlation functions are found to have the same asymptotic behavior in both limits (we drop the subscript y):

$$\langle \mathbf{S}_0\mathbf{S}_R\rangle \sim -\frac{3}{32\pi^2\tilde{Q}}\frac{\exp(-2mR\sqrt{\tilde{Q}/\tilde{P}})}{R^2}\ . \tag{28}$$

The correlation length along the x and y axes, denoted respectively by ξ_x and ξ_y, are given by

$$\xi_x \approx 1/2m$$

and

$$\xi_y \approx (1/2m)\sqrt{P/Q}\ .$$

ξ_y is zero when P vanishes ($J_\perp=0$), which is as expected. We should mention that these asymptotic behaviors are given in the limit where mR is much larger than unity, and all of them are decaying exponentially with the distance R in agreement with the absence of long-range order for this quasi-one-dimensional phase.

IV. CONCLUSION

We have used a SU(N) symmetry bosonic representation based on Schwinger bosons to generalize the SU(2) Heisenberg model for weakly coupled spin chains and searched for a saddle-point solution. It is shown that a phase transition between a disordered phase and an antiferromagnetically ordered one occurs at a finite value of $J_\perp/J$. The dispersion is found to have a finite energy gap Δ in the disordered phase. We know from the mapping onto the O(3) nonlinear σ model that, in the case of one-dimensional systems, the long-wavelength effective action of half integer spin chains possesses an extra topological term while the action of integer spin chains is equivalent to the O(3) nonlinear σ model.[2] This topological term is responsible for the gaplessness of $S=\frac{1}{2}$ spin chains, where the dispersion is calculated exactly.[13] For $S=1$, exact diagonalization[14] and Monte Carlo simulations[15] indicate the existence of an energy gap to the excited state at the wave vector $k=\pi$ which is half of the gap at $k=0$. The Schwinger-boson representation at the mean-field level leads to a gap $\Delta \approx 0.1$ J at both $k=\pi$ and 0.[4] This seems to indicate that corrections beyond the saddle-point approximation are qualitatively important. Clearly, it would be quite interesting to know if incorporating fluctuations can reproduce this ratio of 2 between the gaps at $k=0$ and π.

The energy gap is reduced by the transverse coupling and vanishes at the transition. The asymptotic spin-spin correlation functions are shown to have an exponential decay with the disance in the disordered phase with a correlation length ξ_x or ξ_y depending on the direction. In the x direction we found that ξ_x behaves as $1/\Delta$, which means that ξ_x diverges at the transition. In the y direction ξ_y behaves as $(1/\Delta)\sqrt{P/Q}$ (see Appendix B for the expression of P/Q as a function of $J_\perp/J$). It vanishes as $J_\perp \to 0$ and diverges as $J_\perp$ tends to the critical value.

The model for real experimental $S=1$ systems contains a single-ion anisotropy $D\sum_i (S_i^z)^2$. The values of typical coupling constants are $J_\perp/J \approx 1.7\times 10^{-2}$ and $D/J \approx -0.02$ for $CsNiCl_3$,[16,17] and $J_\perp/J \approx 4\times 10^{-4}$ and $D/J \approx 0.2$ for $Ni(C_2H_8N_2)_2NO_2CPO_4$ (NENP).[18,19] The presence of the D term makes the comparison of our results to experiments difficult. A second difficulty comes from the large S expansion of our calculations, since $S=1$ for the above-mentioned systems. However, we can

draw an interesting conclusion if we ignore the effect of the D anisotropy (this is, of course, unrealistic). It is known that NENP reveals no transition to long-range antiferromagnetic order down to $T=1.2$ K (Ref. 20); we will assume, in order to conclude, that even at $T=0$ K no transition happens. $CsNiCl_3$ gets a transition to 3D long-range order at $T=4.2$ K.[20]

Our estimate of the critical value $J_\perp/J$ from Eq. (17) for $S=1$ is $(J_\perp/J)_c \sim Se^{-2\pi s} \approx 1.86\times10^{-3}$. Sakai and Takahashi[22] give a numerical estimate $(J_\perp/J)_c \approx 1.3\times10^{-3}$ using spin-wave theory as we did in Sec. III A, and another one $(J_\perp/J)_c \approx 0.025$–$0.026$ using a mean-field method in connection with an extrapolation from finite size Lanczos calculation of χ_{st}: $(J_\perp/J)_c = 1/\chi_{st}$, where χ_{st} is the one-dimensional staggered susceptibility. Using our estimates and ignoring D we can place $CsNiCl_3$ and NENP, respectively, in the B (ordered phase) and A (disordered phase) phases of Fig. 2. In the case of $CsNiCl_3$ the single-ion anisotropy will change the predictions because $|D|/J$ and $J_\perp/J$ are of the same order and $D<0$[10] so that at low temperature the energy can be minimized if the z components of the spin are either -1 or $+1$ and not zero. The observed three-dimensional order is clearly due to the effect of both D and $J_\perp$.

The half integer spin case is much less obvious because of the topological term in the long-wavelength effective action. The interchain-coupling tends to enhance long-range order but the topological term, responsible for the gaplessness in the one-dimensional systems, becomes less effective in high dimension.[3,21] A formalism based on fermionic representation[4] for the spin operators gives a power-law decay for the spin-spin correlation function in one dimension, which suggests that it may be relevant for half integer spin S. Clearly, the problem of half integer spins remains quite open.

ACKNOWLEDGMENTS

One of the authors (M.A.) wishes to thank P. Butaud and T. Hsu for helpful discussions.

APPENDIX A

In this appendix, Eq. (14) is derived. Let ω_k be the dispersion relation. The energy gap Δ equals

$$\lambda[1-4(\tilde{Q}+\tilde{P})^2]^{1/2}\ , \tag{A1}$$

where $\tilde{Q}=Q/\lambda$ and $\tilde{P}=P/\lambda$. Equation (12) reduces at $T=0$ K to

$$\frac{2S+1}{\lambda}=\int\frac{d^2k}{(2\pi)^2}\frac{1}{\omega_k}\ , \tag{A2}$$

with

$$\omega_k=\lambda[1-4(\tilde{Q}\cos k_x+\tilde{P}\cos k_y)]^2\ . \tag{A3}$$

Note that the main contributions to the integral of Eq. (A2) come from the center and the corners of the first Brillouin zone, i.e., two points. We shall then expand the cosines and keep only the second orders. Equation (A1) becomes

$$2S+1=\int\frac{d^2k}{(2\pi)^2}\frac{1}{[1-4(\tilde{Q}\cos k_x+\tilde{P}\cos k_y)^2]^{1/2}}\approx 2\int\frac{d^2k}{(2\pi)^2}\frac{1}{[1-4(\tilde{Q}+\tilde{P})^2+4(\tilde{Q}+\tilde{P})(k_x^2\tilde{Q}+k_y^2\tilde{P}]^{1/2}}\ .$$

The factor 2 in front of the integral is here because of the contributions of two points. Using the result of Eq. (13) one gets

$$2S+1\approx\sqrt{2}\int_{-\pi}^{+\pi}\frac{dk_y}{2\pi}\int_{-\pi}^{+\pi}\frac{dk_x}{2\pi}\frac{1}{(\tilde{Q}k_x^2+\tilde{P}k_y^2)^{1/2}}\ .$$

This is then rewritten as

$$2S+1\approx\sqrt{2/\tilde{Q}}\,(1/\pi^2)\int_0^{\pi_y}dk_y\int_0^{\pi\sqrt{(\tilde{Q}/\tilde{P})(1/k_y)}}\frac{du}{(1+u^2)^{1/2}}\ .$$

Using the fact that $\tilde{P}\ll\tilde{Q}$ and then $\tilde{Q}\sim\frac{1}{2}$, we have in the large S limit

$$2S\approx\frac{1}{\pi}\ln\left[\frac{\tilde{Q}}{\tilde{P}}\right]\ ,$$

which implies Eq. (14).

APPENDIX B

This appendix is devoted to the calculation of $\tilde{P}/\tilde{Q}$ and the gap Δ in the one-dimensional limit and the vicinity of the transition. In the one-dimensional limit the integrand is developed in $(P/Q)(1/m^2)$ and calculated in the same spirit as Appendix A. In this case Eq. (12) reads

$$2S+1\approx\frac{1}{\sqrt{\tilde{Q}(\tilde{Q}+\tilde{P})}}\int_0^{\pi}\frac{dk_x}{\pi}\int_0^{\pi}\frac{dk_y}{\pi}\frac{1}{[m^2+k_x^2+(\tilde{P}/\tilde{Q})k_y^2]^{1/2}} \tag{B1}$$

with

$$m^2=\frac{1-4(\tilde{Q}+\tilde{P})^2}{4(\tilde{Q}+\tilde{P})\tilde{Q}} . \tag{B2}$$

After a straightforward calculation one finds

$$2S+1\approx\frac{1}{\tilde{Q}}\left[\frac{1}{\pi}\ln\frac{2\pi}{m}-\frac{\pi}{6}\frac{P}{Q}\frac{1}{m^2}\right] . \tag{B3}$$

Equations (10) and (11) give, in the same way,

$$\frac{Q}{J}\approx\frac{1}{(1+P/Q)^{1/2}}\left[\frac{1}{\pi}\ln\frac{2\pi}{m}-\frac{\pi}{2}-\frac{\pi}{6}\frac{P}{Q}\frac{1}{m^2}-\frac{m^2}{4\pi}-\frac{\pi}{8}\frac{P}{Q}+m^2\ln\frac{2\pi}{m}+\frac{(3-\pi)}{6\pi}\frac{P}{Q}\ln\frac{2\pi}{m}\right] , \tag{B4}$$

$$\frac{P}{J_\perp}\approx\pi\left[\frac{P}{Q}\right]^{1/2}\frac{1}{m} . \tag{B5}$$

The contribution coming from the two-dimensional region in the Brillouin zone dominates in the last equation (B5). The energy gap is estimated to be

$$\Delta\approx 2SJe^{-\pi(S+1/2)}\left\{1-\frac{\pi^4}{384}\left[\left[\frac{e^{\pi(2S+1)}}{2S+1}\right]\frac{J_\perp}{J}\right]^2\right\} . \tag{B6}$$

Using Eqs. (B1), (B2), and (B4), we get

$$\frac{P}{Q}\approx\left[\frac{J_\perp}{\Delta}\right]^2 4\pi^2 , \tag{B7}$$

where we can take the one-dimensional result for Δ ($Je^{-\pi S}$ for large spin S).

Now, in the vicinity of the transition, the small parameter used to expand the integrand is $(P/2)(k_y/m)^2$ for $k_y<(Q/P)m^2$ and $(Q/P)(m/k_y)^2$ for $k_y>(Q/P)m^2$; this allows us to evaluate P/Q and the energy gap. We get

$$\frac{P}{Q}\approx\frac{1}{S+1/2}\frac{J_\perp}{J} , \tag{B8}$$

$$\Delta\sim J\left[\left[\frac{J_\perp}{J}\right]_c-\frac{J_\perp}{J}\right]^{1/2} . \tag{B9}$$

*Present address: Universite de Sherbrooke, Département de Physique et Centre de Recherche en Physique du Solide, Sherbrooke, Québec J1K 2R1, Canada.

[1]T. Kennedy, E. H. Lieb, and B. S. Shastry, J. Stat. Phys. **53**, 108 (1988).
[2]F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983).
[3]F. D. M. Haldane, Phys. Rev. Lett. **61**, 1029 (1988).
[4]D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988).
[5]D. Yoshioka, J. Phys. Soc. Jpn. **58**, 3733 (1989).
[6]P. W. Anderson, Phys. Rev. Lett. **64**, 1839 (1990).
[7]X. G. Wen, Phys. Rev. B **42**, 6623 (1990).
[8]H. J. Schulz, in *Strongly Correlated Electron Systems II,* edited by G. Baskaran, A. E. Ruckenstein, E. Tosatti, and Yu Lu (World Scientific, Singapore, 1991).
[9]The spin-$\frac{1}{2}$ system is gapless in the one-dimensional space. See Ref. 2.
[10]Tôru Sakai and Minoru Takahashi, Phys. Rev. B **42**, 4537 (1990).
[11]N. Read and D. M. Newns, J. Phys. C **16**, 3273 (1983); P. Coleman, Phys. Rev. B **35**, 3702 (1987).
[12]See Refs. 11 for more details.
[13]J. des Cloiseaux and J. J. Pearson, Phys. Rev. **128**, 2131 (1962).
[14]M. Takahashi, Phys. Rev. Lett. **62**, 2313 (1989); Phys. Rev. B **38**, 5188 (1988).
[15]S. V. Meskhov (unpublished).
[16]W. J. L. Buyers, R. M. Mura, R. L. Armstrong, M. J. Hogan, P. Gerlash, and Hirakaiwa, Phys. Rev. Lett. **56**, 371 (1986).
[17]M. Steiner, K. Kakurai, J. K. Kjems, D. Petitgrand, and R. Pynn, J. Appl. Phys. **61**, 3953 (1987).
[18]J. P. Renard, M. Verdaguer, L. P. Regnault, W. A. C. Erkelens, J. Rossat-Mignod, and W. G. Stirling, Europhys. Lett. **3**, 945 (1987).
[19]J. P. Renard, M. Verdaguer, L. P. Regnault, W. A. C. Erkelens, J. Rossat-Mignod, J. Ribas, W. G. Stirling, and C. Vettier, J. Appl. Phys. **63**, 3638 (1988).
[20]L. P. Regnault, J. Rossat-Mignod, J. P. Renard, M. Verdaguer, and C. Vettier, Physica B **156&157**, 247 (1989) and references therein.
[21]T. Dombre and N. Read, Phys. Rev. B **38**, 7181 (1988).
[22]T. Sakai and M. Takahashi, J. Phys. Soc. Jpn. **58**, 3131 (1989).