Interchain-coupling effect on the one-dimensional spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model

Mohamed Azzouz
Centre de Recherche en Physique du Solide et Département de Physique, Université de Sherbrooke, Sherbrooke, Québec, Canada J1K 2R1
(Received 8 April 1993)

Within a mean-field theory, the disordered spin-$\frac{1}{2}$ single-chain state is shown to be unstable towards an antiferromagnetically, long-range ordered one, when any finite transverse coupling, $J_\perp$, is introduced between chains. A mean-field Hamiltonian is derived from the Heisenberg model, using an extension of the Wigner-Jordan transformation in two dimensions. The staggered magnetization and the ground-state energy are calculated for values of transverse couplings ranging from 0 to 1. The main consequence of these calculations is that the value of $J_\perp$, required to have antiferromagnetic long-range order, must only be nonzero. This result is consistent with that of Sakai and Takahashi indicating that the critical transverse coupling should be of order of the inverse of the one-dimensional staggered magnetic susceptibility. Following a qualitative argument, it can also suggest that the Luttinger-liquid state is unstable at least at nearly half-filling for the Hubbard model in the limit of large Coulomb repulsion.

I. INTRODUCTION

The activity in the field of low-dimensional spin systems has been greatly stimulated by the Haldane conjecture.[1] Haldane pointed out that isolated integer-spin chains, with first-nearest-neighbor interaction, have an energy gap in the spin-wave spectrum excitation, whereas the case of half-integer-spin chains is massless. In a previous paper,[2] the effect of a small interchain coupling on a quantum antiferromagnetic two-dimensional array of spin chains in the case of integer spin is studied. In this work the case of the spin $S=\frac{1}{2}$ is investigated. For integer spin the correlation length is finite and the spin-spin correlation decreases exponentially with the distance. For $S=\frac{1}{2}$ the correlation function decreases algebraically as $1/R$, implying an infinite correlation length. This difference in behavior is attributed to the presence of a topological term in the long-wavelength action of spin-$\frac{1}{2}$ chains and not in the action of integer-spin chains.[1] Consequently, for integer spin a finite transverse coupling $J_\perp$ is required to establish long-range antiferromagnetic order.[2] The case of half-integer spin is more difficult. This is due to the simultaneous disappearance of the topological term[3] and the decrease of the quantum spin fluctuations, as soon as the transverse coupling becomes nonzero. We can expect that the system would become massive once $J_\perp$ is nonzero and that, to have long-range order, a finite transverse coupling would be required as in the case of integer spins. But the results of this work suggest that the system gets ordered for any finite transverse coupling. This result has been found out already by Sakai and Takahashi,[4] who combined a mean-field treatment with a one-dimensional exact diagonalization. However, the originality of our present work is that the method, applied here, is entirely analytic and allows the calculation of the local magnetization for any value of $J_\perp$. Because of the mean-field approximation, the result we obtain, for the magnetization in the isotropic two-dimensional Heisenberg model, is found to be greater than the one given by spin-wave analysis.

On the other hand, the discovery of high-critical-temperature superconductors[5] has lead to the interesting question of whether a Luttinger-liquid state can occur or not in more than one dimension.[6] Our results may suggest that the Luttinger liquid is unstable toward another state in more than one dimension, at least at nearly half-filling for the Hubbard model in the case of large Coulomb repulsion U. We know from renormalization-group analysis that this is equally true for the small-U limit.[7] The Hubbard model is canonically equivalent to the Heisenberg model for large U and at half-filling. Let us assume that we create a single hole on one chain. If the chains are decoupled, then we get a Luttinger liquid. Now, if a transverse coupling is switched on, the hole will not be able to distabilize the long-range order, because we need a finite density of holes to disorder the system.[8] The Luttinger liquid is unstable in the sense that we get an ordered spin system for any finite transverse coupling.

In this work we introduce a generalization of the Wigner-Jordan transformation in two dimensions. In order to do so, we recall briefly the one-dimensional Wigner-Jordan transformation which allows a mapping of the XY model into a spinless free-fermion Hamiltonian. Then the anisotropic two-dimensional Heisenberg model is mapped, within this transformation, to interacting spinless fermions. These fermions are moving in a gauge field generated by the spin configuration itself. A flux-phase Néel ground-state type is found to give, at the mean-field level, the lowest variational energy, for all finite transverse couplings.

II. METHOD AND RESULTS

The Hamiltonian of the XY model is given by

$$H_{xy}=J\sum_{\langle i,j\rangle}\{S_i^xS_j^x+S_i^yS_j^y\}\ , \tag{1}$$

with the sum running only over the first nearest neighbors $\langle i,j \rangle$. J is a positive antiferromagnetic exchange constant. In one dimension this model is exactly solvable using the Wigner-Jordan transformation[9]

$$S_i^z = c_i^+ c_i - \tfrac{1}{2} ,$$
$$S_i^- = c_i \exp\left[i\pi \sum_{j=0}^{i-1} n_j \right] , \tag{2}$$
$$n_j = c_j^+ c_j .$$

The commutation relations of the spin operators are satisfied since we consider that c_i and c_i^+ apply to fermions. The presence of the phase of S_i^- in Eq. (2) is essential in preserving these commutation relations when they are calculated for two different sites. The commutator

$$[S_i^-, S_j^-] = c_i \exp\left[i\pi \sum_{k=0}^{i-1} n_k \right] c_j \exp\left[i\pi \sum_{k=0}^{j-1} n_k \right] - c_j \exp\left[i\pi \sum_{k=0}^{j-1} n_k \right] c_i \exp\left[i\pi \sum_{k=0}^{i-1} n_k \right] , \tag{3}$$

where $i < j$ without lose of generality, vanishes since the important relation

$$e^{i\pi n_i} c_i = -c_i e^{i\pi n_i} \tag{4}$$

holds for any site i. Next, we present schematically the transformation (2) as is indicated in Fig. 1, where the dashed line shows that to obtain the phase of S_i^- we summed up from the site 0 to $i-1$, in the phase of the expression of S_i^-(2). It is important to note that this summation does not extend to every site, except i, in order to preserve the spin commutation relations.

In one dimension the commutator $[S_i^-, S_j^-]$ with j greater than i, as shown in Fig. 2, equals zero because the operator c_i appears once and only once, multiplied by the phase term $e^{i\pi n_i}$ of Eq. (2), in the products $S_i^- S_j^-$ and $S_j^- S_i^-$. To indicate that $c_i e^{i\pi n_i}$ appears only once, only one dashed line crosses the site i in Fig. 2. If we make use of (4), we then will be able to get $[S_i^-, S_j^-] = 0$. This idea is very helpful to obtain a generalization of the Wigner-Jordan transformation in the case of two dimensions. The question is reduced to how to make a generalization of the one-dimensional scheme.

Following Eq. (2), the up or down spins correspond to the absence or presence of one fermion, respectively. H_{xy} becomes a spinless free-fermion Hamiltonian

$$H_{xy} = \frac{J}{2} \sum_i c_i^\dagger c_{i+1} + \text{H.c.} , \tag{5}$$

with a Fermi surface half-filled. But in the presence of a transverse coupling between chains, the problem gets too

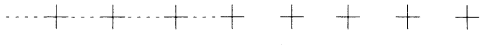

FIG. 1. Dashed line indicates that, to obtain the phase in the transformation (2) at the site i, we summed on the occupation number of all the sites from the origin until $i-1$.

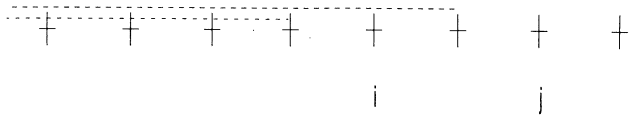

FIG. 2. Dashed line crosses only one time the site i. This is to say that $\pm e^{i\pi n_i}$ appears only once in the products of the commutators between i and j.

complicated to be solved by the one-dimensional Wigner-Jordan transformation, because the commutation relations are no longer satisfied and because the XY model can no longer be mapped into a free-fermion Hamiltonian. To surmount the first difficulty, we introduce a generalization of the Wigner-Jordan transformation by proceeding in the same spirit as for the exactly one-dimensional problem. We propose a transformation where the phase at the site (i,j) is, now, obtained by summing up all the sites at the left of the dashed line as indicated in Fig. 3.[10] The summation contains also the sites belonging to the dashed line. Two coordinates i and j are taken, respectively, on the x and y axes to specify a given site. The extended transformation is defined as

$$S_{i,j}^- = c_{i,j} \exp\left\{ i\pi \left[\sum_{d=0}^{i-1} \sum_{f=0}^{\infty} n_{d,f} + \sum_{f=0}^{j-1} n_{i,f} \right] \right\} ,$$
$$S_{i,j}^z = c_{i,j}^\dagger c_{i,j} - \tfrac{1}{2} , \tag{6}$$

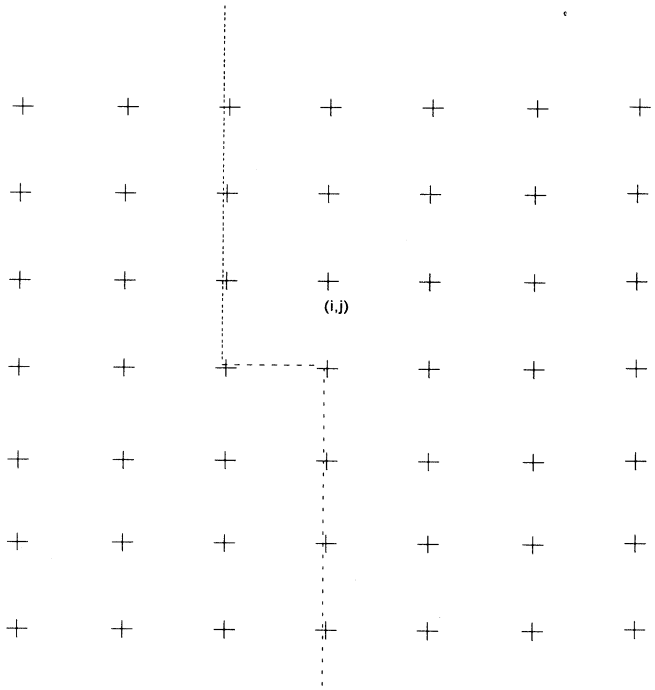

FIG. 3. We summed up all the sites, located at the left of the dashed line, to get the phase of the lowering spin operator at the site (i,j): Eq. (10). The sites belonging to this line are contained in the summation. Using the same reasoning as in Fig. 2, it is not hard to convince ourselves that the commutation relations are preserved.

where the operator $c_{i,j}$ takes two space indices i and j. It is possible to show, following the same reasoning as before, that the commutation relations are preserved. This transformation gives explicitly the phase of $S^-_{i,j}$, which is a complicated function of the configuration of spins in the considered region. Wang[11] has proposed a similar transformation, but with the difference that he did not specify the phase as we did. Other extensions of the Wigner-Jordan transformation in two dimensions appear in the literature.[12] Using this transformation, the two-dimensional XY model becomes

$$H_{xy}=\frac{J}{2}\sum_{i,j,\delta} c_{i,j}e^{-i\phi_{i,i+\delta}(j)}c^{\dagger}_{i+\delta,j} + \frac{J_\perp}{2}\sum_{i,j,\delta} c_{i,j}e^{-i\varphi_{j,j+\delta}(i)}c^{\dagger}_{i,j+\delta}\ , \tag{7}$$

which is an effective hopping Hamiltonian for fermions, moving in a gauge field created by the spin configuration itself. $J_\perp$ is, as J, a positive exchange constant in the y direction. The hopping of the fermions is between nearest neighbors, and the hopping amplitudes are

$$\frac{J}{2}e^{-i\phi_{i,i+\delta}(j)} \tag{8}$$

in the x direction and

$$\frac{J_\perp}{2}e^{-i\varphi_{j,j+\delta}(i)} \tag{9}$$

in the y direction. The phases $\phi_{i,i+\delta}(j)$ and $\varphi_{j,j+\delta}(i)$ are as follows:

$$\phi_{i,i+\delta}(j)=\delta\pi\left\{\sum_{f=j}^{\infty} n_{i-\delta_{i-1,i+\delta},f}+\sum_{f=0}^{j-1} n_{i+\delta_{i+1,i+\delta},f}\right\}, \qquad \varphi_{j,j+\delta}(i)=\delta\pi n_{i,j-\delta_{j-1,j+\delta}}\ . \tag{10}$$

In these formulas, $\delta_{j\pm1,j+\delta}$ is the Kronecker symbol, and $\delta=\pm1$ indicates the first nearest neighbors of a given site. The operator $n_{i,j}$ is the occupation number at the site (i,j). These two phases are not symmetrical because of the choice of the gauge in the transformation (6). Every site is occupied by either an up or down spin, corresponding to the presence or absence of a fermion as in one dimension. Therefore these phases have a nonobvious dependence on the fermions positions. If $J_\perp=0$, then the one-dimensional limit is recovered by using a Read-Newns gauge transformation,[13] where $c_{i,j}$ is transformed into $c_{i,j}e^{i\theta_{i,j}}$ with $\theta_{i,j}=-\sum_{n<i}\phi_{n,n+1(j)}$.

This calculation shows how the XY model becomes difficult to analyze in two dimensions, whereas it has an obvious solution in one dimension. The asymmetrical form of the phases ϕ and φ allows us, however, to get a state similar to the known mean-field solution of the uniform flux-phase state.[14] We see that ϕ can be either 0 or π depending on the spin configuration, and so it may have on average (it is a statistical average) a value of $\pi/2$. φ is then equal to zero as in the one-dimensional problem. The dispersion relation is calculated assuming a bipartite lattice:

$$E(\mathbf{k})=\pm(J^2\sin^2k_x+J_\perp^2\cos^2k_y)^{1/2}\ . \tag{11}$$

This dispersion relation is not symmetric in k_x and k_y. But an another gauge, where k_x is replaced by k_y in (11) and vice versa, is also possible and we can show that our results are gauge invariant [see Eq. (23) below]. It becomes quite clear that the uniform flux-phase solution is a very good candidate to represent the ground state of the XY model in two dimensions.

Now the Heisenberg model is expressed, in the following way, using Eqs. (6) and (7):

$$H=H_{xy}+J\sum_{i,j,\delta} n_{i,j}n_{i+\delta,j}+J_\perp\sum_{i,j,\delta} n_{i,j}n_{i,j+\delta}\ . \tag{12}$$

H represents interacting spinless fermions. The second and third terms measure repulsive interactions J and $J_\perp$ between fermions belonging to adjacent sites. Equation (12) has the advantage of not needing any constraint on the fermion occupation number. The Fermi statistics of the operators ensures no double occupancy. It is interesting to compare this Hamiltonian with that of the Schwinger-boson analysis.[2,15] As was done by Wang[11] in the case of an isotropic two-dimensional Heisenberg model, we search for a Hartree-Fock solution for the term biquadratic in fermion annihilation and creation operators. The decoupling of this term takes into account two tendencies in the physics of the problem. The first one is characterized by the presence of a flux-phase term, and the second one is the result of the assumption of long-range antiferromagnetic order. The dispersion relation, calculated in the gauge discussed above, is

$$E_\pm(\mathbf{k})=\pm[(J+J_\perp)^2m^2+J^2(1+2Q)^2\sin^2k_x + J_\perp^2(1+2P)^2\cos^2k_y]^{1/2}\ , \tag{13}$$

where $m=|\langle n_{i,j}\rangle|$, $Q=|\langle c_{i,j}c^{\dagger}_{i+1,j}\rangle|$, and $P=|\langle c_{i,j}c^{\dagger}_{i,j+1}\rangle|$ are three variational parameters. m is the local magnetization, and Q and P are interpreted as effective hopping terms in the x and y directions respectively. It is interesting to note that, for a similar phase to (13), Hsu[16] showed that spin-wave excitations are allowed. In our approach this can be done by calculating Gaussian corrections which give a particle-particle-type interaction between quasiparticles in the lower band. This is beyond the scope of the present work. The presence of the gap $2(J+J_\perp)m$ at $(k_x,k_y)=(0,\pm\pi/2)$ is an "insulating gap" and is interpreted as the energy required to flip a spin (create a quasiparticle and quasihole pair which corresponds to the creation of a domain-wall excitation in the space of the spins). This behavior is not seen in the case of the XY model, where the gap is zero. It becomes obvious that the gap will vanish once the long-range order disappears in the case of the Heisenberg model when the system gets away from half-filling. We are interested in studying only the ground-state properties. The values of the variational parameters are determined by minimizing the total energy with respect to m, Q, and P. This gives, at zero temperature, a set of three self-consistent equations

$$m=\int\frac{d^2k}{(2\pi)^2}\frac{(J+J_\perp)}{E_+(\mathbf{k})}m\ , \tag{14}$$

$$Q=\frac{1}{2}\int\frac{d^2k}{(2\pi)^2}\frac{J\sin^2k_x}{E_+(\mathbf{k})}(1+2Q)\ , \tag{15}$$

$$P=\frac{1}{2}\int\frac{d^2k}{(2\pi)^2}\frac{J_\perp\cos^2k_y}{E_+(\mathbf{k})}(1+2P)\ . \tag{16}$$

We will search for a nonzero magnetization m since the corresponding energy is lower than that of $m=0$. First, we are interested in the limit where $J_\perp$ is much smaller than J. We are going to calculate m when $J_\perp$ is exactly zero and show that this limit is singular. The reason is that in one dimension the local magnetization is zero[17] and the ground state has no long-range antiferromagnetic order. Putting $J_\perp=0$ in Eqs. (14)–(16) leads to

$$m=\int_{-\pi}^{+\pi}\frac{dk_x}{2\pi}\frac{1}{[m^2+(1+2Q)^2\sin^2k_x]^{1/2}}m\ , \tag{17}$$

$$Q=\frac{1}{2}\int_{-\pi}^{+\pi}\frac{dk_x}{2\pi}\frac{\sin^2k_x}{[m^2+(1+2Q)^2\sin^2k_x]^{1/2}}(1+2Q)\ , \tag{18}$$

where $m=0$ is a solution of (17) and it implies $Q=1/\pi$ from (18). But as we mentioned above, the total energy can be minimized further by a nonvanishing solution of m. In this way we get

$$m=\frac{2}{\pi}\frac{1}{(1+\alpha^2)}K\left[\frac{\alpha}{(1+\alpha^2)^{1/2}}\right]\ , \tag{19}$$

$$Q=\frac{1+2Q}{\pi m\alpha^2}\left\{(1+\alpha^2)^{1/2}E\left[\frac{\alpha}{(1+\alpha^2)^{1/2}}\right]-m\frac{\pi}{2}\right\}\ , \tag{20}$$

where $\alpha=(1+2Q)/m$. We see that m must be of order of unity to avoid the divergence of Eq. (18). K and E are the complete elliptic integrals of, respectively, the first and second kind. If we assume that m is very small compared to $1+2Q$, then we get rough estimations of

$$Q\approx\frac{1}{\pi} \tag{21}$$

and

$$m\approx 4(1+2Q)e^{-(1+2Q)\pi/2}\approx 0.5\ . \tag{22}$$

These values of m and Q are confirmed approximately by a numerical solution of (17) and (18) ($m=0.513$ and $Q=0.285$).

Equations (14)–(16) are solved numerically for any value of the transverse coupling. In Fig. 4 we plot the variation of m and see that it is an increasing function of $J_\perp/J$. The local magnetization m is 0.778 for the isotropic model. This estimation is, of course, higher than the spin-wave one (0.6) (a value of $m=1$ is the full sublattice magnetization). This discrepancy is due to the mean-field treatment which underestimates quantum fluctuations. Still, from Fig. 4, it is seen that the one-dimensional limit is singular, because we know from exact results that the antiferromagnetic chain is disordered ($m=0$). We calculate the ground-state energy and plot it in Fig. 5 for various values of the transverse coupling and for $m>0$. This energy is compared with the one we get by considering

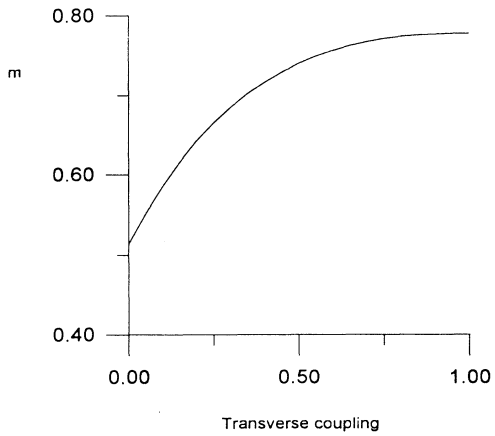

FIG. 4. Staggered magnetization, calculated in the Hartree-Fock approximation, is plotted as a function of the transverse coupling.

the $m=0$ solution. The reduction of the energy separation between these two levels ($m>0$ and $m=0$), as the transverse coupling is decreased, is a signature of the fact that the quantum fluctuations become stronger and stronger with decreasing the transverse coupling. So, in our mean-field approximation, a transition between disorder and antiferromagnetic order occurs at a critical value of the transverse coupling, $J_\perp=0$. This result is consistent with the one found by Sakai and Takahashi.[4] A finite critical value of the transverse coupling would manifest itself by producing a crossover between the levels $m=0$ and $m>0$ at a nonzero value of $J_\perp$. In Fig. 6 we draw the variations of Q, P, and P/Q as functions of $J_\perp/J$. In all these figures, J is set equal to unity. In order to see the gauge invariance, we have performed a calculation with the energy spectrum

$$E_\pm(\mathbf{k})=\pm[(J+J_\perp)^2m^2+J^2(1+2Q)^2\cos^2k_x+J_\perp^2(1+2P)^2\sin^2k_y]^{1/2} \tag{23}$$

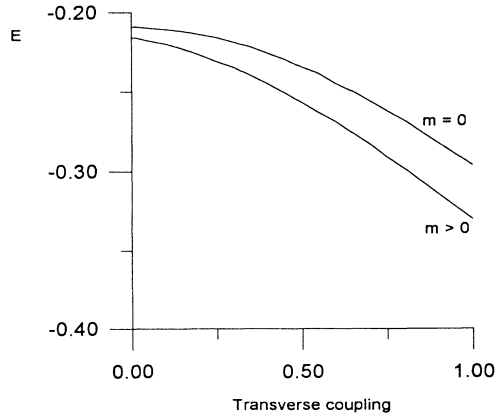

FIG. 5. Energy vs transverse coupling. The $m>0$ curve is the ground-state energy. This energy is compared with the one calculated for the $m=0$ solution of the self-consistent equations [Eqs. (14)–(16)].

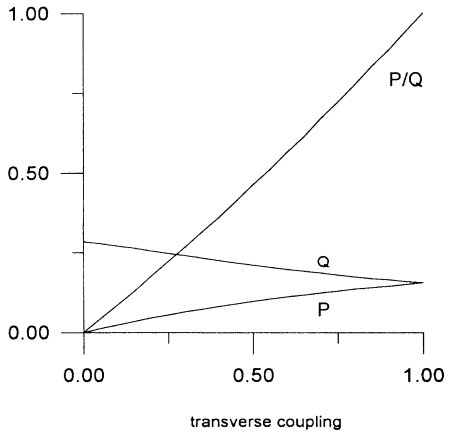

FIG. 6. Mean-field parameters Q, P, and P/Q vs transverse coupling for $m>0$. P/Q nearly behaves as $J_\perp/J$.

and found the same results for m, Q, and P.

When holes are introduced by doping the system, the situation becomes different. We expect that for any concentration of holes smaller than the critical value δ_c, where the antiferromagnetic order disappears for $J_\perp>0$, our result would remain qualitatively exact, and the one-dimensional Luttinger liquid is destroyed for any finite transverse coupling. To explain this we develop the following argument. Assume that a single hole is created on one chain in a system where all chains are decoupled. What we get is a Luttinger liquid with a charge-spin separation. If, now, these chains are coupled within a transverse coupling $J_\perp$, then the system will undergo a transition to an ordered phase, because the single hole will not be able to destroy long-range order. Things are certainly complicated for doping greater than δ_c.

III. CONCLUSION

Weakly coupled Heisenberg spin-$\frac{1}{2}$ chains are studied in this work. Within a simple mean-field approximation, it is found that the critical value of the transverse coupling, required to have long-range antiferromagnetic order, is equal to zero. This result is in contrast with the case of integer spin. In this case it is almost established that a finite critical value is necessary to undergo a transition between the one-dimensional disordered phase and the two-dimensional ordered one. The correction beyond the mean-field solution may be important in the limit of small $J_\perp$. The question of Gaussian fluctuations is planned to be addressed in an upcoming work.

ACKNOWLEDGMENTS

Part of this work was done at the "Centre de Recherches sur les Très Basses Températures" in Grenoble. I acknowledge its financial support. Discussions with B. Doucot, T. Dombre, A.-M. S. Tremblay, and C. Bourbonnais have been most helpful.

[1]F. D. M. Haldane, Phys. Lett. **93A**, 463 (1983); Phys. Rev. Lett. **50**, 1153 (1983).
[2]M. Azzouz and B. Doucot, Phys. Rev. B **47**, 8660 (1993).
[3]F. D. M. Haldane, Phys. Rev. Lett. **61**, 1029 (1988).
[4]T. Sakai and M. Takahashi, J. Phys. Soc. Jpn. **58**, 3131 (1989).
[5]J. G. Bednorz and K. A. Muller, Z. Phys. B **64**, 188 (1986).
[6]P. W. Anderson, Phys. Rev. Lett. **64**, 1839 (1990); X. G. Wen, Phys. Rev. B **42**, 6623 (1990).
[7]C. Bourbonnais and L. G. Caron, Int. J. Mod. Phys. B **5**, 1033 (1991).
[8]Several works shows that the two-dimensional Heisenberg systems remain antiferromagnetically ordered when one single hole is introduced at half-filling; see, for example, G. Martinez and P. Horsh, Phys. Rev. B **44**, 317 (1991).
[9]E. H. Leib, T. Shultz, and D. J. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).
[10]This transformation was introduced by M. Azzouz, Ph.D. thesis, Université Joseph Fourier-Grenoble 1, France, 1992.
[11]Y. R. Wang, Phys. Rev. B **43**, 3786 (1991).
[12]See, for example, J. Ambjorn and G. Semenoff, Phys. Lett. B **226**, 107 (1989); E. Fradkin, Phys. Rev. Lett. **63**, 322 (1989).
[13]N. Read and D. M. Newns, J. Phys. C **16**, 3272 (1983).
[14]I. Affleck and J. B. Marston, Phys. Rev. B **37**, 316 (1988).
[15]D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 3733 (1989).
[16]T. C. Hsu, Phys. Rev. B **41**, 11 379 (1990).
[17]Spin-wave theory supports this result. See, for example, P. W. Anderson, Phys. Rev. **86**, 694 (1952).