Generalization of the Jordan-Wigner transformation in three dimensions and its application to the Heisenberg bilayer antiferromagnet

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We extend the definition of the Jordan-Wigner transformation to three dimensions using the generalization of ideas that were introduced in the two-dimensional case by one of the present authors. Under this transformation, the three-dimensional XY spin Hamiltonian is mapped onto a system of spin-less fermions coupled to a gauge field with only two nonzero components. This gauge field is calculated explicitly. Then we apply this transformation to the investigation of the Heisenberg bilayer antiferromagnet. The interesting quantum disordered state realized in this material for strong interlayer couplings is studied in detail. We define the physical parameter that governs this state, and calculate analytically several quantities, such as the ground-state energy and the energy gap as a function of the interlayer coupling. Very good agreement with existing results and with the infinite interlayer coupling limit is recovered.

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I. INTRODUCTION

Jordan and Wigner[1] introduced a transformation that maps local spin-1/2 operators, S^- and S^z, to Fermi operators in one dimension. For example, this transformation leads to the mapping of the one-dimensional XY Hamiltonian onto a Hamiltonian of noninteracting spin-less fermions. Trying to generalize this result in two dimensions proved to be difficult. Several authors have given implicit ways of defining such a generalization in two dimensions.[2,3] But, a natural extension of the Jordan-Wigner (JW) transformation was introduced by one of the present authors[4] to study the interchain-coupling effect on the one-dimensional spin-1/2 Heisenberg antiferromagnets. The generalization of the JW transformation has been attempted even in three dimensions by Huerta and Zanelli[5] who introduced an implicit transformation, by Kochmański[6] whose transformation, however, does not preserve some of the spin-commutation relations, and by Shaofeng[7] who erred in two claims as will be discussed in Sec. III.

The JW transformations are applied in such areas as quantum field theory, statistical mechanics of quantum and classical systems, and in the physics of phase transitions and critical effects. A pretty application of the one-dimensional transformation in condensed matter physics is the solution to the two-dimensional Ising model by Schultz, Mattis and Lieb.[8] This transformation is very useful for studying quantum spin systems. Our aim in this work is to find a generalization of the JW transformation in three dimensions where the phase of the transformation is given explicitly in terms of fermion number operators, and to shed light on one particular unclear point of such a generalization, that is the flux-per-plaquette as one fermion moves around this plaquette.

Then we apply the three-dimensional JW transformation to the Heisenberg bilayer quantum antiferromagnet in order to support the validity of our findings. Once the Heisenberg Hamiltonian on the bilayer is written in terms of the spin-less JW fermions, the bond-mean-field theory approach[4,9–11] is used in order to decouple the interacting terms. In the past, several bosonic-type approaches[12–16] have been used to study this system. At zero temperature, the Heisenberg bilayer antiferromagnet presents a disordered gaped state for strong interlayer coupling, known as the disordered quantum state, but an antiferromagnetically ordered state for weak coupling. A second order quantum phase transition takes place between these two states at a critical value of the interlayer coupling. The bilayer quantum antiferromagnet may be of some relevance to some of the high temperature superconductors in their low-doping normal state.[12,17] One of our aims here is to provide a full description of the disordered quantum state at zero temperature in terms of one or several physical parameters. Not only we were able to accomplish that, but the mean-field equations of the present approach can be solved analytically in this state.

This paper is organized as follows. In Sec. II, the generalized transformation is introduced. In Sec. III, the phase change per plaquette is calculated in the context of the XY Hamiltonian. The application of our findings to the Heisenberg bilayer antiferromagnet is made in Sec. IV. Summary and conclusions are drawn in the last section.

II. THE THREE-DIMENSIONAL JW TRANSFORMATION

Generalizing the ideas that led to the introduction of the two-dimensional JW transformation,[4] allowed us to define the transformation in three dimensions by

$$S^-_{i,j,k}=c_{i,j,k}e^{i\pi\phi_{i,j,k}},$$

$$S^z_{i,j,k}=c^\dagger_{i,j,k}c_{i,j,k}-1/2, \tag{1}$$

$$\phi_{i,j,k}=\sum_{\epsilon=0}^{k-1}\sum_{\alpha=0}^{\infty}\sum_{\beta=0}^{\infty}n_{\alpha,\beta,\epsilon}+\sum_{\alpha=0}^{i-1}\sum_{\beta=0}^{\infty}n_{\alpha,\beta,k}+\sum_{\beta=0}^{j-1}n_{i,\beta,k}.$$

Here, $n_{i,j,k}=c^{\dagger}_{i,j,k}c_{i,j,k}$ is the number operator of the spin-less fermions; $c^{\dagger}_{i,j,k}$ and $c_{i,j,k}$ being the creation and annihilation operators of a spin-less fermion at site (i,j,k), respectively. The phase may be written in a simpler form by borrowing the notations of Shaofeng[7] who attempted to generalize the JW transformation in three dimensions, but erred in two points (please see below):

$$\phi(\mathbf{x})=\sum_{z=0}^{\infty} w(\mathbf{x},\mathbf{z})n(\mathbf{z}), \tag{2}$$

where

$$\begin{aligned} w(\mathbf{x},\mathbf{z})=&\Theta(x_3-z_3)(1-\delta_{x_3,z_3})+\Theta(x_1-z_1)\delta_{x_3,z_3}\\ &\times(1-\delta_{x_1,z_1})+\Theta(x_2-z_2)\delta_{x_1,z_1}\delta_{x_3,z_3}\\ &\times(1-\delta_{x_2,z_2}), \end{aligned} \tag{3}$$

a result that is different from the one of Shaofeng[7] in which the $(1-\delta_{x_2,z_2})$-factor in the last term is missing. This constitutes the first of the two errors made by Shaofeng. This factor is essential for preserving spin commutation relations. The condition $e^{i\pi w(\mathbf{x},\mathbf{z})}=-e^{i\pi w(\mathbf{z},\mathbf{x})}$ that is necessary to preserve nonlocal spin commutation relations is satisfied by Eq. (3). We also explicitly checked that all possible combinations of spin commutation relations are preserved. To obtain the phase (2) we choose a plane going through the site where we want to define the transformation. Here the plane (0,0,1) is chosen. Then we sum over those sites on this plane as in the two-dimensional transformation.[4] Finally we sum over all sites that are behind this plane. $\mathbf{x}=(x_1,x_2,x_3)$ and $\mathbf{z}=(z_1,z_2,z_3)$ stand for sites on a cubic lattice for simplicity.

III. THE PHASE PER PLAQUETTE

Consider the XY model written for a three-dimensional array of coupled layers:

$$\begin{aligned} H_{XY}=&\frac{J}{2}\sum_{i,j,k} S^{-}_{i,j,k}S^{+}_{i+1,j,k}+\frac{J}{2}\sum_{i,j,k} S^{-}_{i,j,k}S^{+}_{i,j+1,k}\\ &+\frac{J_{\perp}}{2}\sum_{i,j,k} S^{-}_{i,j,k}S^{+}_{i,j,k+1}+(\text{H.c.}), \end{aligned} \tag{4}$$

where J and $J_{\perp}$ are, respectively, the intralayer and interlayer coupling constants, and (H.c) stands for the Hermitian conjugate of all terms in Eq. (4). Under the JW transformation (1), Hamiltonian (4) is mapped onto a Hamiltonian of spin-less fermions:

$$\begin{aligned} H_{XY}=&\frac{J}{2}\sum_{i,j,k} c^{\dagger}_{i,j,k}c_{i+1,j,k}e^{i\partial_i\phi_{i,j,k}}+\frac{J}{2}\sum_{i,j,k} c_{i,j+1,k}e^{i\pi n_{i,j,k}}c^{\dagger}_{i,j,k}\\ &+\frac{J_{\perp}}{2}\sum_{i,j,k} c^{\dagger}_{i,j,k}c_{i,j,k+1}e^{i\partial_k\phi_{i,j,k}}+(\text{H.c}). \end{aligned} \tag{5}$$

Here $\partial_i\phi_{i,j,k}=\phi_{i+1,j,k}-\phi_{i,j,k}$ and $\partial_k\phi_{i,j,k}=\phi_{i,j,k+1}-\phi_{i,j,k}$ designate discrete derivatives along the x and z axes, respectively. According to Fradkin,[2] this effective Hamiltonian describes the motion of spin-less fermions coupled to a gauge field. A very important cancellation takes place in the second term of Eq. (5) namely, $c_{i,j+1,k}c^{\dagger}_{i,j,k}e^{i\pi n_{i,j,k}}=c^{\dagger}_{i,j,k}c_{i,j+1,k}$ because $e^{i\pi n_{i,j,k}}c^{\dagger}_{i,j,k}\equiv -c^{\dagger}_{i,j,k}$. For this reason, there is no phase attached to the hopping of a spin-less fermion along the y axis. Let the site-dependent gauge field components be $A_i(i,j,k)=\partial_i\phi_{i,j,k}$ along the x axis, $A_j(i,j,k)=\partial_j\phi_{i,j,k}$ along the y axis, and $A_k(i,j,k)=\partial_k\phi_{i,j,k}$ along the z axis. This leads to

$$\begin{aligned} A_i&=\pi\left[\sum_{\beta=0}^{\infty} n_{i,\beta,k}+\sum_{\beta=0}^{j-1}(n_{i+1,\beta,k}-n_{i,\beta,k})\right],\\ A_j&=0,\\ A_k&=\pi\left[\sum_{\alpha=0}^{i-1}\sum_{\beta=0}^{\infty}(n_{\alpha,\beta,k+1}-n_{\alpha,\beta,k})+\sum_{\beta=0}^{j-1}(n_{i,\beta,k+1}-n_{i,\beta,k})\right.\\ &\quad\left.+\sum_{\alpha=0}^{\infty}\sum_{\beta=0}^{\infty} n_{\alpha,\beta,k}\right]. \end{aligned} \tag{6}$$

The effective magnetic field is obtained through the discrete curl of $\mathbf{A}$, namely $\mathbf{B}(i,j,k)=\boldsymbol{\nabla}\times\mathbf{A}(i,j,k)$ [the vectors $\mathbf{A}$ and $\mathbf{B}$ depend on the position (i,j,k)]. The site-dependent components of $\mathbf{B}$ are therefore given by

$$\begin{aligned} B_i&=\pi(n_{i,j,k+1}-n_{i,j,k}),\\ B_j&=0,\\ B_k&=\pi(n_{i,j,k}-n_{i+1,j,k}). \end{aligned} \tag{7}$$

Hence the effective magnetic field to which the spin-less fermions couple presents two nonzero components only. Note that the indices i, j, and k in the components of A and B refer to the directions along axes x, y, and z. This magnetic field satisfies $\boldsymbol{\nabla}\cdot\mathbf{B}=\partial_iB_i+\partial_jB_j+\partial_kB_k=0$, a result that excludes the existence of monopoles in consistency with Maxwell equations, and with $\mathbf{B}=\boldsymbol{\nabla}\times\mathbf{A}$; $\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\times\mathbf{A})=0$. Note that the vector potential $\mathbf{A}$ and the magnetic field $\mathbf{B}$ are operators in the present problem, not simple numbers as in the classical electromagnetic theory.

As for the phase change that occurs when a spin-less fermion completes a motion around a plaquette, we consider the elementary plaquettes in the xy, xz, and yz planes. Let a spin-less fermion move around a plaquette in the context of the XY model: when the fermion moves in the x and z axes, phase differences occur, whereas when it moves along the y axis the phase difference is zero. The flux per plaquette in the xy plane turns out to be the same as in two dimensions, that is

$$\Phi_{xy}=\pi(n_{i,j,k}-n_{i+1,j,k}). \tag{8}$$

For a spin-less fermion starting its motion at site (i,j,k), $n_{i,j,k}=1$. Then for this fermion to go to site $(i+1,j,k)$, this later site has to be empty due to Pauli exclusion principle; thus $n_{i+1,j,k}=0$. In this approximation one

finds that the phase is π, which is consistent with the mean-field result.[3] Finally, for a plaquette in the yz plane the result is

$$\Phi_{yz}=\pi(n_{i,j,k+1}-n_{i,j,k}). \tag{9}$$

Similarly, the phase per plaquette can be set to be approximately π. As for the phase around the plaquette in the xz plane, it is found to be identically zero:

$$\Phi_{xz}=0. \tag{10}$$

It is worth noting here that the results of the fluxes per plaquette obtained in Eqs. (8), (9), and (10), are consistent with the expressions of magnetic field components in Eqs. (7) (the unit area being $a^2=1$), namely that $\Phi_{xy}=\int \mathbf{B}\cdot d\mathbf{a}=B_k a^2=B_k \ldots$. The results for the above fluxes-per-plaquette imply that as a spinless fermion moves around a given plaquette, it will couple to a gauge field if the plaquette belongs to plane xy or yz, but no coupling to a gauge field occurs in the remaining plane xz.

Shaofeng[7] mistakenly reported that the phase change around any elementary plaquette is zero. The reason for obtaining this incorrect result is that this author did not take into account the fact that $S^-_{i,j+1,k}S^+_{i,j,k}$ transforms into $c_{i,j+1,k}e^{i\pi n_{i,j,k}}c^\dagger_{i,j,k}\equiv c^\dagger_{i,j,k}c_{i,j+1,k}$ [which transforms the second term in Eq. (5) to a free hopping of the spin-less fermions along the y axis] because $e^{i\pi n_{i,j,k}}c^\dagger_{i,j,k}\equiv -c^\dagger_{i,j,k}$. This constitutes the second error made by Shaofeng in attempting to generalize the JW transformation.

IV. APPLICATION TO THE HEISENBERG BILAYER ANTIFERROMAGNET

A. Description of the approach

In the second part of this paper, we apply the above transformation to the investigation of the Heisenberg bilayer antiferromagnet that has received a lot of attention in the past few years.[12–22] The use of the JW transformation and the bond-mean-field theory[4,9] does not need a constraint on the occupation number as required in the Schwinger boson approach,[12,18,19] modified spin-wave approaches,[15] or the bond-operator mean-field theory.[21,22] However, the present fermionic approach suffers from the difficulty related to treating the effect of the phase terms. Here, these are treated in mean-field theory. We would like to draw the attention to the bond-mean field approach[4,9] which has so far given very satisfactory results in the case of the Heisenberg ladder.[10,11]

The Heisenberg model on a bilayer reads as follows:

$$H=H_{XY}+J\sum_{i,j,k} S^z_{i,j,k}S^z_{i+1,j,k}+J\sum_{i,j,k} S^z_{i,j,k}S^z_{i,j+1,k}+J_\perp\sum_{i,j,k} S^z_{i,j,k}S^z_{i,j,k+1}, \tag{11}$$

which transforms to

$$H=H_{XY}+J\sum_{i,j,k}\left(c^\dagger_{i,j,k}c_{i,j,k}-\frac{1}{2}\right)\left(c^\dagger_{i+1,j,k}c_{i+1,j,k}-\frac{1}{2}\right)+J\sum_{i,j,k}\left(c^\dagger_{i,j,k}c_{i,j,k}-\frac{1}{2}\right)\left(c^\dagger_{i,j+1,k}c_{i,j+1,k}-\frac{1}{2}\right)+J_\perp\sum_{i,j,k}\left(c^\dagger_{i,j,k}c_{i,j,k}-\frac{1}{2}\right)\left(c^\dagger_{i,j,k+1}c_{i,j,k+1}-\frac{1}{2}\right) \tag{12}$$

when transformation (1) is used. Hamiltonian (12) is simplified using the approximation where the average flux per elementary plaquette is π on the xy and yz planes [as discussed below Eqs. (8) and (9)]. The flux phase is identically zero on elementary plaquettes in the xz plane. We stress that this approximation is the same as what is obtained in mean-field theory calculation.[3] We choose the following configuration: the phases are alternated $\ldots\pi-0-\pi-0\ldots$ along the adjacent bonds on the y axis, and zero on all bonds on the remaining axes. Note that the alternated phases could be put rather on the x axis without changing the physical results because of gauge invariance. However, in the case of the bilayer system, the alternated phases cannot be put on the z axis because there is only one bond along that axis.

Further simplification is done using the bipartite character due to antiferromagnetic correlations. Two types of fermions $c^A_{i,j,k}$ on sublattice A and $c^B_{i',j',k'}$ on sublattice B, where (i',j',k') is one of the adjacent sites of (i,j,k), are introduced. Then we decouple the interacting quartic terms by introducing the alternated magnetization parameter $m_{i,j,k}=2\langle S^z_{i,j,k}\rangle=2\langle c^\dagger_{i,j,k}c_{i,j,k}\rangle-1=m(-1)^{i+j+k}$, and the bond parameters $Q=\langle c_{i,j,k}c^\dagger_{i+1,j,k}\rangle=\langle c_{i,j,k}c^\dagger_{i,j+1,k}\rangle$ within the layers and $P=\langle c_{i,j,k}c^\dagger_{i,j,k+1}\rangle$ perpendicular to the layers. Parameters Q and P are assigned the same phase distribution as above, namely $\ldots\pi-0-\pi\ldots$ along the x axis and zero on the rest of the bonds along y and z axes. Q and P are taken to be distinct parameters as the coupling constants within the layers and between the layers are different, and because of the geometry of the bilayer. Both Q and P represent the same physical quantity in two different directions. But, P plays a far more crucial role than Q in the occurrence of the quantum transition, and the stabilization of the disordered quantum state as will be shown later in this paper. We use the following approximation:

$$\mathcal{O}\mathcal{O}'\approx\langle\mathcal{O}\rangle\mathcal{O}'+\langle\mathcal{O}'\rangle\mathcal{O}-\langle\mathcal{O}\rangle\langle\mathcal{O}'\rangle, \tag{13}$$

which neglects fluctuations around the mean-field point $\langle\mathcal{O}\rangle$ and $\langle\mathcal{O}'\rangle$ because we assume that $(\mathcal{O}-\langle\mathcal{O}\rangle)(\mathcal{O}'-\langle\mathcal{O}'\rangle)\approx 0$, a result that leads to Eq. (13). $\mathcal{O}$ and $\mathcal{O}'$ are any two operators. Using approximation (13) with $\mathcal{O}=S_{i,j,k}$ and $\mathcal{O}'=S_{i+1,j,k}$, $S_{i,j+1,k}$, or $S_{i,j,k+1}$ on one hand, and $\mathcal{O}=c_{i,j,k}c^\dagger_{i+1,j,k}$, $c_{i,j,k}c^\dagger_{i,j+1,k}$, or $c_{i,j,k}c^\dagger_{i,j,k+1}$, and $\mathcal{O}'=\mathcal{O}^\dagger$ on the other hand gives the following approximate form for H:

$$H=J\sum_{i,j,k}\frac{m}{2}(e^{\dagger}_{2i,2j,2k}e_{2i,2j,2k}-f^{\dagger}_{2i+1,2j,2k}f_{2i+1,2j,2k})+J\sum_{i,j,k}\frac{m}{2}(e^{\dagger}_{2i+1,2j+1,2k}e_{2i+1,2j+1,2k}-f^{\dagger}_{2i,2j+1,2k}f_{2i,2j+1,2k})$$
$$+J\sum_{i,j,k}\frac{m}{2}(e^{\dagger}_{2i+1,2j+1,2k}e_{2i+1,2j+1,2k}-f^{\dagger}_{2i+1,2j,2k}f_{2i+1,2j,2k})+J\sum_{i,j,k}\frac{m}{2}(e^{\dagger}_{2i,2j,2k}e_{2i,2j,2k}-f^{\dagger}_{2i,2j+1,2k}f_{2i,2j+1,2k})$$
$$+J_{\perp}\sum_{i,j,k}\frac{m}{2}(e^{\dagger}_{2i,2j,2k}e_{2i,2j,2k}-f^{\dagger}_{2i,2j,2k+1}f_{2i,2j,2k+1})+J_{\perp}\sum_{i,j,k}\frac{m}{2}(e^{\dagger}_{2i+1,2j,2k+1}e_{2i+1,2j,2k+1}-f^{\dagger}_{2i+1,2j,2k}f_{2i+1,2j,2k})$$
$$+\frac{J_1}{2}\sum_{i,j,k}(e^{\dagger}_{2i,2j,2k}f_{2i+1,2j,2k}-f^{\dagger}_{2i+1,2j,2k}e_{2i+2,2j,2k})+\text{H.c.}+\frac{J_1}{2}\sum_{i,j,k}(e^{\dagger}_{2i,2j,2k}f_{2i,2j+1,2k}+f^{\dagger}_{2i,2j+1,2k}e_{2i,2j+2,2k})+\text{H.c.}$$
$$+\frac{J_{\perp 1}}{2}\sum_{i,j,k}(e^{\dagger}_{2i,2j,2k}f_{2i,2j,2k+1}+f^{\dagger}_{2i,2j,2k+1}e_{2i,2j,2k+2})+\text{H.c.}+N\left(\frac{2J+J_{\perp}}{4}m^2+2JQ^2+J_{\perp}P^2\right), \tag{14}$$

where J_1 and $J_{\perp 1}$ are defined by

$$J_1=J(1+2Q),$$
$$J_{\perp 1}=J_{\perp}(1+2P), \tag{15}$$

and $e_{i,j,k}=c^A_{i,j,k}$ (respectively $f_{i,j,k}=c^B_{i,j,k}$) is the fermion operator on sublattice A (respectively B). Now, Q and P stand for their own moduli. Here, $N=N_xN_yN_z$ is the total number of sites; $N_x=N_y$ being the number of sites along the x and y axes, and N_z the number of sites along the z axis. Hamiltonian (14) is written for a unit cell which is a cube of side $a=1$ where sites are labeled by $(2i,2j,2k)$, $(2i+1,2j,2k)$ along the x axis, $(2i,2j,2k)$, $(2i,2j+1,2k)$ along the y axis, and $(2i,2j,2k)$, $(2i,2j,2k+1)$ along the z axis. In Fourier space, we define $e_{\mathbf{k}}$ and $f_{\mathbf{k}}$ as the Fourier transforms of operators c^A and c^B respectively: $c^A_{i,j,k}=\Sigma_{\mathbf{k}<}e_{\mathbf{k}}e^{-i\mathbf{r}^A_{i,j,k}\cdot\mathbf{k}}/\sqrt{N/2}$ and $c^B_{i,j,k}=\Sigma_{\mathbf{k}<}f_{\mathbf{k}}e^{-i\mathbf{r}^B_{i,j,k}\cdot\mathbf{k}}/\sqrt{N/2}$. The summation $\Sigma_{\mathbf{k}<}$ runs over half the original Brillouin zone because the direct space unit cell volume has doubled due to antiferromagnetic sublattices. Accordingly, the Hamiltonian takes the simpler form:

$$H=\sum_{\mathbf{k}<}M(e^{\dagger}_{\mathbf{k}}e_{\mathbf{k}}-f^{\dagger}_{\mathbf{k}}f_{\mathbf{k}})+\sum_{\mathbf{k}<}[iJ_1\sin k_x+\gamma(k_y,k_z)]e^{\dagger}_{\mathbf{k}}f_{\mathbf{k}}$$
$$+\text{H.c.}+N\left(\frac{2J+J_{\perp}}{4}m^2+2JQ^2+J_{\perp}P^2\right), \tag{16}$$

where

$$\gamma(k_y,k_z)=J_1\cos k_y+J_{\perp 1}\cos k_z,$$
$$M=(2J+J_{\perp})m.$$

The first two terms in Eq. (16) are results of the decoupling procedure using the local parameter m, whereas the second term and its Hermitian conjugate describe the hopping of JW fermions between adjacent sites due to the XY term of Eq. (12) and to the decoupling procedure using the nonlocal bond parameters Q and P. Along the x axis, the hopping amplitude is $-i\sin k_x$ because of the phase configuration $\ldots\pi-0-\pi-0\ldots$. This term is obtained by Fourier transforming the first term in J_1 of Eq. (14). Along the two remaining axes, the hopping is of tight-binding type with amplitude $\gamma(k_y,k_z)$.

B. Mean-field equations and the energy spectrum

Hamiltonian (16) is transformed into the diagonal form

$$H=\sum_{\mathbf{k}<}E(\mathbf{k})[\alpha^{\dagger}_{\mathbf{k}}\alpha_{\mathbf{k}}-\beta^{\dagger}_{\mathbf{k}}\beta_{\mathbf{k}}] \tag{17}$$

after defining the quasiparticle operators $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ by

$$\alpha_{\mathbf{k}}=u^*_{\mathbf{k}}e_{\mathbf{k}}+v_{\mathbf{k}}f_{\mathbf{k}},$$
$$\beta_{\mathbf{k}}=v^*_{\mathbf{k}}e_{\mathbf{k}}-u_{\mathbf{k}}f_{\mathbf{k}}, \tag{18}$$

where $u_{\mathbf{k}}=e^{i\eta_{\mathbf{k}}/2}\cos\theta_{\mathbf{k}}$ and $v_{\mathbf{k}}=e^{i\eta_{\mathbf{k}}/2}\sin\theta_{\mathbf{k}}$, with $\cos\theta_{\mathbf{k}}=\{[M+E(\mathbf{k})]/2E(\mathbf{k})\}^{1/2}$ and $\tan\eta_{\mathbf{k}}=J_1\sin k_x/\gamma(k_y,k_z)$. $E(\mathbf{k})$ and $\Gamma(\mathbf{k})$ are given by

$$E(\mathbf{k})=[M^2+|\Gamma(\mathbf{k})|^2]^{1/2},$$
$$\Gamma(\mathbf{k})=\gamma(k_y,k_z)+iJ_1\sin k_x. \tag{19}$$

The ground state corresponds to the situation where the lower band described by β is full and the upper band described by α is empty. The chemical potential for the JW fermions is zero. Therefore the ground-state energy is given by

$$E_{\mathrm{GS}}=\frac{(2J+J_{\perp})m^2}{4}+2JQ^2+J_{\perp}P^2-\frac{1}{N}\sum_{\mathbf{k}}\frac{E(\mathbf{k})}{2}, \tag{20}$$

where $\Sigma_{\mathbf{k}}\equiv\Sigma_{k_x,k_y,k_z}$ now holds on the original Brillouin zone because the factor 1/2 in the summation term takes care of the fact that we had to sum over half the Brillouin zone. Because we use periodic boundary conditions, $k_i=n_i2\pi/N_i$ with $i=x,y,z$ and $n_i=0,1,\ldots,N_i-1$. For the bilayer ($N_z=2$) periodic boundary conditions count $J_{\perp}$ twice. Thus, we

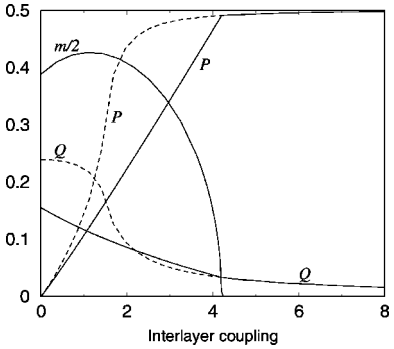

FIG. 1. The parameters m, Q and P are plotted as a function of $J_\perp$. Full lines are obtained by allowing m to be nonzero, whereas dashed lines are for the solution $m=0$. Magnetization vanishes at $J_{\perp c}=4.2J$.

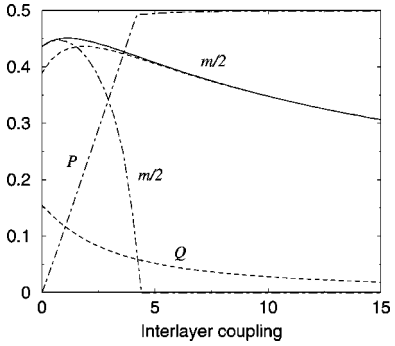

FIG. 2. The magnetization $m/2$ is displayed as a function of $J_\perp$ in the case where the bond parameters $Q=0$ and $P=0$ (full line), $P=0$ and $Q\neq 0$ (dashed line), and $Q=0$ and $P\neq 0$ (dashed-dotted line).

have to multiply by 2 the value of $J_\perp$ in all final results or divide $J_\perp$ by 2 in all our equations.

The parameters m, Q, and P are calculated self-consistently through the equations

$$m=\frac{1}{N}\sum_{\mathbf{k}} m(2J+J_\perp)/E(\mathbf{k}),$$

$$Q=\frac{1}{N}\sum_{\mathbf{k}} \{J_1\sin^2 k_x+\gamma(k_y,k_z)\cos k_y\}/4E(\mathbf{k}), \quad (21)$$

$$P=\frac{1}{N}\sum_{\mathbf{k}} \gamma(k_y,k_z)\cos k_z/2E(\mathbf{k}),$$

obtained by minimizing the ground-state energy with respect to m, Q and P: $\partial E/\partial Q=\partial E/\partial P=\partial E/\partial m=0$. Next we analyze these equations.

C. Physical parameters P, Q, and m

The set of self-consistent equations (21) consist of integral equations that cannot be solved analytically in general. It is only in the strong coupling regime that we are able to solve them analytically as we do in the next subsection. For now, we seek a solution numerically using a numerical iterative method. The results of such a calculation are depicted in Fig. 1 for Q, P, and m as functions of the interlayer coupling $J_\perp$. When $J_\perp$ increases, P increases and approaches 0.5, whereas Q decreases to 0. The magnetization $m/2$ vanishes at $J_\perp\equiv J_{\perp c}=4.2J$, thus marking the onset of a second order transition from the antiferromagnetic state for $J_\perp<J_{\perp c}$ to the quantum disordered state for $J_\perp>J_{\perp c}$. In the antiferromagnetic state, the values assumed by Q and P are different from those that would be assumed if the state were not ordered. Interestingly, the presence of Q and P reduces the value of m for if these bond parameters were not considered, the magnetization would be greater than what it is now. To understand this point and the effects inducing the quantum transition, we study the following situations where only some of the mean-field parameters are considered at once.

When we decouple the interaction terms of Hamiltonian (12) using parameter m alone, the magnetization (full line in Fig. 2) does not vanish. This implies that the quantum transition does not take place. When decoupling is done using parameters m and Q only, m does not vanish either (dashed line in Fig. 2). Finally, when decoupling is performed using parameters m and P only, magnetization vanishes signaling the occurrence of the quantum transition (dashed-dotted line in Fig. 2). Thus, this transition is switched on by the bond parameter P. Parameter Q plays a (minor) role in the reduction of magnetization $m/2$ for values of $J_\perp\leqslant J_{\perp c}$.

D. Analytical solution of the mean-field equations in the strong limit, $J_\perp/J_{\perp c}>1$

We define the strong coupling regime by $J_\perp/J_{\perp c}>1$. The mean-field equations (21) can be solved approximately in the disordered state. In the particular case of the limit $J_\perp/J\sim\infty$, which is realized by setting $J=0$, an exact solution is possible:

$$m=0, \quad Q=0, \quad P=\frac{1}{2}\sum_{k_z=0,\pi}\frac{|\cos k_z|}{2}=\frac{1}{2} \quad (22)$$

because $E(\mathbf{k})=J_{\perp 1}|\cos k_z|=J_{\perp 1}$; $k_z=0$, π. The result $P=1/2$ for $J=0$ is consistent with the numerical result reported in Fig. 1, namely that when $J_\perp/J\to\infty$, $P\to 1/2$. Next, in the limit $J_\perp>J_{\perp c}$, the energy spectrum can be expanded as follows:

$$E(\mathbf{k})=[J_1^2\sin^2 k_x+\gamma^2(k_y,k_z)]^{1/2}$$
$$\approx J_{\perp 1}\left[1+\frac{J_1}{J_{\perp 1}}\cos k_y\cos k_z+\frac{1}{2}\frac{J_1^2}{J_{\perp 1}^2}\sin^2 k_x\right] \quad (23)$$

and approximating the integrals in Eq. (21) by their values near band minima leads to

$$P\approx\frac{1}{2}, \quad Q\approx\frac{J_1}{8J_{\perp 1}}, \quad m=0, \quad (24)$$

which gives

$$P\approx\frac{1}{2}, \quad Q\approx\frac{J}{8J_\perp-2J}, \quad m=0 \quad (J_\perp\gg J), \quad (25)$$

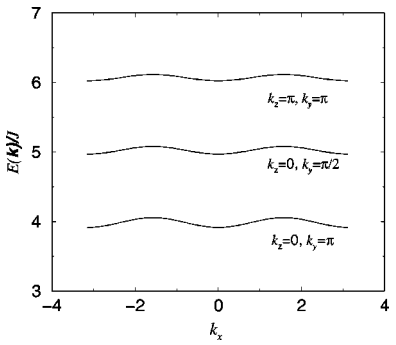

FIG. 3. The energy spectrum $E(\mathbf{k})$ is displayed along the x axis for some values of k_y and for $k_z=0,\ \pi$. The interlayer coupling is $J_\perp=5J$. The energy gap is realized at $(k_x,k_y,k_z)=(k_0,\pi,0)$ in the bottom band ($k_0=0,\ \pi$); $E_g\approx 4J$ consistently with Eq. (30): $E_g \approx 5J-J=4J$.

once Eq. (15) is used. Equation (23) indicates that for large $J_\perp/J$, $E(\mathbf{k})$ shows little dispersion along the x axis as the coefficient of the leading term that depends on k_x is at most $(J/J_\perp)^2$. In Fig. 3, $E(\mathbf{k})$ is displayed using Eq. (19) along the x axis for several values of k_y and k_z. Note the little dispersion in k_x. The set of solutions (25), which agree very well with the numerical results reported in Fig. 1, will be used in the discussion of the disordered quantum state in the next section.

E. The disordered quantum state; $m=0$

The second order transition takes place due to the fact that the symmetries of the ground states for weak and strong coupling regimes are different. On one hand, for infinite interlayer coupling $J_\perp/J\sim\infty$, the system consists of $N/2$ decoupled singlets where rotation invariance is preserved. On the other hand, for $J_\perp=0$, both layers of spins are ordered antiferromagnetically at $T=0$, and rotational invariance is broken. Therefore as $J_\perp$ increases, a transition from the magnetically ordered state to the disordered state occurs, Fig. 1. The disordered state is a gaped state in which the energy spectrum is given by Eq. (23), and $u_\mathbf{k}=v_\mathbf{k}=e^{i\eta_\mathbf{k}}/\sqrt{2}$ because $M=(2J+J_\perp)m=0$. The energy gap at $\mathbf{k}=(k_0,\pi,0)$ or $(k_0,0,\pi)$, k_0 being $=0$ or π, is given by

$$E_g=|J_{\perp 1}-J_1|=|J_\perp(1+2P)-J(1+2Q)|, \qquad (26)$$

if $J_{\perp 1}>J_1$. The later condition is deduced by setting $\gamma(k_y,k_z)=0$ which is essential for a vanishing gap. Numerically we find that the value above which an energy gap opens is $J_\perp=2\times 0.78J=1.56J$, see Sec. IV E 3 below. However, this does not mean that this is the critical value for the order-disorder second-order quantum transition.

1. Physical parameter P

The mean-field parameter that suitably governs this state is $\langle S^-_{i,j,1}S^+_{i,j,2}\rangle\approx-\langle c_{i,j,1}c^\dagger_{i,j,2}\rangle=-P$ which describes how a pair of spins on adjacent sites belonging to different layers are locked into a spin singlet. The ground state consists of the formation of such $N/2$ spin singlets. As Figs. 1 and 2 show, P is, for all practical purposes, 1/2 for $J_\perp>J_{\perp c}$, a result that indicates that the spin singlets are very robust because they are able to keep their strength ($P\approx 1/2$) for all couplings between $J_\perp/J=4.2$ up to infinity.

2. Ground state and ground-state energy

The infinite $J_\perp$ limit is worth considering here in order to understand the quantum disorder state. In this case $u_\mathbf{k}=v_\mathbf{k}=1/\sqrt{2}$, and the quasiparticle operators reduce to

$$\alpha_\mathbf{k}\equiv\frac{1}{\sqrt{2}}(c_1+c_2),$$

$$\beta_\mathbf{k}\equiv\frac{1}{\sqrt{2}}(c_1-c_2), \qquad (27)$$

where c_1 and c_2 are JW annihilation operators on respectively adjacent sites where each one belongs to one layer. The ground state consists of creating a quasi-particle β:

$$\beta^\dagger_\mathbf{k}|0,0\rangle=\frac{1}{\sqrt{2}}(c^\dagger_1-c^\dagger_2)|0,0\rangle=\frac{1}{\sqrt{2}}(|1,0\rangle-|0,1\rangle)$$

$$=\frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle), \qquad (28)$$

as occupation by a spinless fermion means the presence of spin up, and its absence means the presence of spin down, or vice versa. Clearly, this is the spin singlet that constitutes the ground state of a pair of spins interacting antiferromagnetically.

As for the ground-state energy, one finds

$$E_{\rm GS}=J_\perp\langle\mathbf{S}_{i,j,1}\cdot\mathbf{S}_{i,j,2}\rangle$$

$$=J_\perp\left[\langle S^z_{i,j,1}S^z_{i,j,2}\rangle+\frac{1}{2}(\langle S^+_{i,j,1}S^-_{i,j,2}\rangle+\langle S^-_{i,j,1}S^+_{i,j,2}\rangle)\right]$$

$$\approx-3J_\perp/4,$$

because $\langle S^z_{i,j,1}S^z_{i,j,2}\rangle=\langle S^y_{i,j,1}S^y_{i,j,2}\rangle=\langle S^x_{i,j,1}S^x_{i,j,2}\rangle$ due to rotational invariance, and $\langle S^+_{i,j,1}S^-_{i,j,2}\rangle\simeq-1/2$. Note that $-3J_\perp/4$ is the energy of the spin-singlet state (28). The fact that the limit $J_\perp/J\sim\infty$ is well described by the present approach is very promising. It seems to indicate that coupled singlets (J finite) will be described at least as well because mean-field theory is supposed to work better for a large number of degrees of freedom.

In the strong limit, we use the same approximation as in Sec. IV D. The ground-state energy $E_{\rm GS}$ is found to be

$$E_{\rm GS}\approx 2JQ^2+J_\perp P^2-\frac{1}{2}J_{\perp 1}\left(1+\frac{J_1^2}{J_{\perp 1}^2}\right), \qquad (29)$$

where Q and P are given by Eq. (24). Equation (29) yields corrections to the singlet ground-state energy to all orders in $J/J_\perp$. It is found that Eq. (29) compares well with the numerical results as shown in Fig. 4. The later not only displays the results of our calculation for $E_{\rm GS}$ obtained numerically using Eq. (20), as a function of $J_\perp$, but also the results

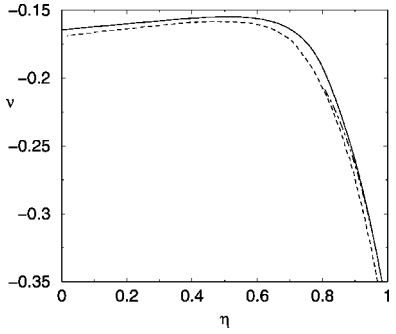

FIG. 4. The ground-state energy as defined by ν is plotted as a function of the reduced interlayer coupling as defined by η. The dashed line is from Ref. 20. The dashed-dotted line (plotted for $J_\perp > J_{\perp c}$) is the result of Eq. (30).

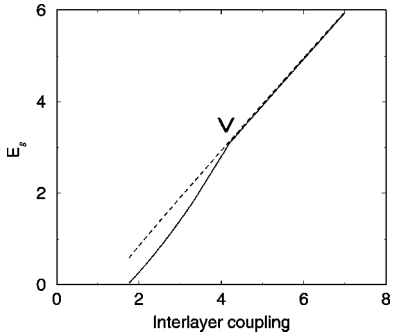

FIG. 5. The result of the energy gap E_g obtained numerically is drawn as a function of $J_\perp$ (full line). Comparison is made to the result of expression (30), which is obtained in the strong limit (dashed line). Notice that the agreement is very good in the disordered quantum state for which $J_\perp > 4.2J$ as shown by v. Interestingly, the gap is nonzero in the antiferromagnetic state for $1.56J < J_\perp < 4.2J$, a fact that indicates that the singlet retains some kind of existence even when it is not the predominant factor in determining the symmetry of the ground state.

reported by Weihong[20] obtained using Ising expansion and dimer expansion. The quantity $\nu = E_{\rm GS}/(4J + J_\perp)$ is drawn as a function of $\eta = J_\perp/(J + J_\perp)$. The maximum of ν at $\eta = 0.5$ coincides with that reported by Weihong, and in general both results agree very well.

3. Energy gap

Breaking a spin singlet requires an energy E_g as given by Eq. (26). Deep in the disordered quantum state, i.e., for $J_\perp/J_{\perp c} \gg 1$, $E_g \simeq J_\perp(1+2P) \approx 2J_\perp$ which gives $E_g \simeq J_\perp$ once double counting of $J_\perp$ due to the periodic boundary conditions is discarded. In this limit, the gap is consistent with the energy separation between the lower and higher levels of the single $(J=0)$ spin pair, that is $J_\perp/4 - (-3J_\perp/4) = J_\perp$. Near the critical point $J_{\perp c}$, Using Eq. (26), the correction to the gap due to intralayer coupling J reads as

$$E_g \approx J_\perp - J - \frac{J^2}{4J_\perp - J} \quad (J_\perp \gg J) \tag{30}$$

because P and Q are given by Eq. (25). Equation (30) gives the correction to the energy gap to all orders in $J/J_\perp$. Figure 5 displays the results of the numerical calculations and their comparison with Eq. (30). It turns out that the agreement between them is very satisfactory, to say the least.

F. Elementary excitations in the disordered state

Using Eq. (18), sublattice operators $e_{\mathbf{k}}$ and $f_{\mathbf{k}}$ can be written in terms of quasi-particle operators, $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$, as

$$e_{\mathbf{k}} = u_{\mathbf{k}}(\alpha_{\mathbf{k}} + \beta_{\mathbf{k}}),$$
$$f_{\mathbf{k}} = u^*_{\mathbf{k}}(\alpha_{\mathbf{k}} - \beta_{\mathbf{k}}). \tag{31}$$

The energy $E(\mathbf{k})$ represents the spectrum of elementary excitations in the system. At zero temperature, the lower band is fully occupied whereas the upper band is empty. In the language of JW spin-less fermions, elementary excitations consist of creating particle-hole pairs only. This is realized by annihilating a JW fermion in the lower band and creating a fermion in the upper one. Creating a particle alone, or a hole alone, violates the conservation of JW fermions, since the number of particle operator $\mathcal{N} = \Sigma_{\mathbf{k}<}(e^\dagger_{\mathbf{k}} e_{\mathbf{k}} + f^\dagger_{\mathbf{k}} f_{\mathbf{k}})$ $= \Sigma_{\mathbf{k}<}(\alpha^\dagger_{\mathbf{k}}\alpha_{\mathbf{k}} + \beta^\dagger_{\mathbf{k}}\beta_{\mathbf{k}})$ commutes with Hamiltonian (17): in terms of spin variables this translates to $dS^z_{Tot}/dt = 0$, which implies the conservation of the total z component of the spin. As a consequence, there appears a selection rule on the sectors of the total z component of the spin that can be connected by elementary excitations: only $|\mathrm{GS}, S^z_{Tot}=0\rangle \rightarrow |\mathrm{ES}, S^z_{Tot}=0\rangle$ excitations are possible because the ground state is a singlet. GS and ES designate the ground state and an excited state respectively. In the limit $J_\perp/J \sim \infty$, the excited state is

$$\alpha^\dagger_{\mathbf{k}}\beta_{\mathbf{k}}[\beta^\dagger_{\mathbf{k}}|0,0\rangle] = \frac{1}{\sqrt{2}}(c^\dagger_1 + c^\dagger_2)|0,0\rangle = \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle) \tag{32}$$

which is one of the triplet states with $S_{Tot}=1$ and $S^z_{Tot}=0$. In the strong coupling limit, $J_\perp \gg J$, $u_{\mathbf{k}} = 1/\sqrt{2} + O(J/J_\perp)$. Therefore, up to a correction of order $J/J_\perp$ elementary excitations will continue to consist of singlet-triplet excitations as in the infinite limit $J_\perp/J \sim \infty$. Overall, the quantum disordered state is very well described by the bond-mean-field theory.

G. Antiferromagnetic state; $m \neq 0$

The zero magnetization solution is stable only for $J_\perp > J_{\perp c}$ as Fig. 1 shows. The phase is ordered antiferromagnetically for $J_\perp < J_{\perp c}$. The value $J_{\perp c} = 4.2J$ compares well to the result $(4.48J)$ of the Schwinger boson approach[12,18,19] and that of the spin-wave theory.[15] But it disagrees with the Monte Carlo simulations[14] result $(2.5J)$ or the series expansion[17] calculation $(2.56J)$. Chubokov and Morr[15] reported that while transverse spin-wave excitations are gapless (Goldstone modes) longitudinal spin-wave excitations are gapped for $J_{\perp c} > J_\perp > 0$. Our result seems to indicate that a finite value of the interlayer coupling $(J_\perp = 1.56J)$ would be needed for the longitudinal fluctuations to become relevant. Note however that we have to consider Gaussian fluc-

tuations about our mean-field point to account for spin-wave excitations in the ordered phase. This would possibly lead to a better estimate of the critical point $J_{\perp c}$. Figure 1 shows that the magnetization increases with $J_{\perp}$, passes through a maximum, then decreases in agreement with previous results.[15]

V. CONCLUSION

In summary, this work dealt with extending the definition of the JW transformation in three dimensions and its application to the Heisenberg bilayer antiferromagnet. Under this transformation, the three-dimensional Heisenberg model transforms into a system of interacting spinless fermions that are coupled to a gauge field for which the magnetic field is a two-component vector operator (one of the three component being zero). The magnetic field satisfies Maxwell equations ruling out the possibility of the existence of monopoles in three-dimensional Heisenberg systems. The flux per plaquette is nonzero for two of the three elementary perpendicular plaquettes, but is zero for the third one. These findings are applied to the study of the Heisenberg bilayer antiferromagnet in the framework of the bond-mean field approach. We recalculated the order-disorder critical coupling, the ground-state energy, and the energy gap.

Furthermore, the disordered state is investigated in detail. The nature of the ground state is reported to be consisting of coupled singlets formed by spins on adjacent sites belonging to different layers. The dominant parameter that governs this state is found to be simply given by $P \approx |\langle S^{-}_{i,j,1} S^{+}_{i,j,2} \rangle|$. P is shown to be responsible for the onset of the quantum disordered state. Good agreement with limiting cases ($J_{\perp} \rightarrow 0$ and $J_{\perp} \rightarrow \infty$), and with results from previous studies is obtained. The present fermionic approach is consistent with the bosonic-type approaches, namely the spin-wave theory and the Schwinger boson method. Not only the generalization of the Jordan-Wigner transformation, introduced in this paper, is rigorous from the mathematical point of view, but it also leads to very satisfactory results for the Heisenberg bilayer antiferromagnet. A fact that indicates that it is physically sound as well.

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