# Numerical Jordan-Wigner approach for two-dimensional spin systems

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We present a numerical self-consistent variational approach based on the Jordan-Wigner transformation for two-dimensional spin systems. We apply it to the study of the well-known quantum (S=1/2) antiferromagnetic XXZ system as a function of the easy-axis anisotropy  $\Delta$  on a periodic square lattice. For the SU(2) case the method converges to a Néel ordered ground state irrespective of the input density profile used and in accordance with other studies. This shows the potential utility of the proposed method to investigate more complicated situations such as frustrated or disordered systems.

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### I. INTRODUCTION

Quantum spin systems in two-dimensional (2D) lattices have been the subject of intense research, mainly motivated by their possible relevance in the study of high-temperature superconductors. On the other hand, high-magnetic-field experiments on materials with a 2D structure which can be described by the Heisenberg antiferromagnetic model in frustrated lattices have revealed novel phases as plateaux and jumps in the magnetization curves.<sup>2</sup> In spite of the huge efforts made, a general understanding of the phase diagram of such magnets is elusive and it is then worth trying to develop new techniques to study these systems systematically. Among the many different techniques that have been used to study such systems, the generalization of the celebrated Jordan-Wigner (JW) transformation<sup>3</sup> to two spatial dimensions<sup>4</sup> has some appealing features. It allows one to write the spin Hamiltonian completely in terms of spinless fermions in such a way that the S = 1/2 single-particle constraint is automatically satisfied due to the Pauli principle, while the magnetic field enters as the chemical potential for the JW fermions. The price one has to pay is the appearance of complicated nonlocal interactions between fermions. This method has been applied in Ref. 5 (see also Ref. 6) to study the XXZ Heisenberg antiferromagnet. These studies have been reviewed in Ref. 7.

More recently this technique was used to obtain a theoretical magnetization curve for the Shastry-Sutherland model, reproducing at the mean-field (MF) level some of the experimentally observed features for the material SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub> which is assumed to be described by such model. Also the  $J_1$ - $J_2$  model, in relation to  $\text{Li}_2\text{VOSiO}_4$  and  $\text{Li}_2\text{VOGeO}_4$  compounds, and the XY model were analyzed with the same technique. All the studies performed have been based on a mean-field decoupling scheme as the starting point to deal with the nonlocal interactions introduced by the JW transformation. In Ref. 5 the mean-field procedure was further supplemented by the inclusion of fluctuations in terms of an auxiliary gauge field with a leading Chern-Simons dynamics coupled to the lattice fermions. However, in spite of the partial success of the JW transformation, many problems remain open, in particular in connection to the study of frustrated systems such as the triangular lattice. In some cases, the results obtained via a direct meanfield treatment lead to results that are believed to be incorrect, such as the appearance of a spin gap in the triangular lattice case (see the discussion in Ref. 8). The main problem associated with the JW approach is related to the implementation of the above-mentioned mean-field decoupling, which renders the description approximate. Another highly nontrivial problem is the construction of the lattice description of the Chern-Simons theory, which has been carefully studied for the square lattice case only.<sup>11</sup>

It is the purpose of the present paper to propose a systematic self-consistent mean-field method for exploring the ground state (g.s.) of 2D lattice spin- $\frac{1}{2}$  systems, in a way that could be applied to arbitrary lattice topologies. The method can also be used in the presence of an external magnetic field, at finite temperature and even be applied to disordered systems.

# II. JORDAN-WIGNER TRANSFORMATION IN TWO DIMENSIONS

The Jordan-Wigner transformation in two spatial dimensions was originally proposed in Ref. 4 as a generalization of the well-known transformation in 1D, and has been further developed in Refs. 5, 6. It maps a set of spin- $\frac{1}{2}$  operators  $\tilde{S}_{p}$ on lattice sites p into spinless fermion operators  $c_p$  by

$$S_{p}^{-} = c_{p} \exp \left[ i \sum_{q \neq p} \theta_{qp} c_{q}^{\dagger} c_{q} \right],$$

$$S_{p}^{+} = c_{p}^{\dagger} \exp \left[ -i \sum_{q \neq p} \theta_{qp} c_{q}^{\dagger} c_{q} \right],$$

$$S_{p}^{z} = c_{p}^{\dagger} c_{p} - 1/2, \tag{1}$$

where  $S^{\pm} = S^x \pm iS^y$  are the usual spin raising and lowering operators and  $\theta_{qp}$  is the argument of the vector drawn from site p to site q. The transformation is nonlocal, and sets a preferred quantization axis z. The spin operators (1) satisfy bosonic SU(2) commutation relations, while the Pauli principle ensures that they belong to the irreducible representation S=1/2. Indeed, the only necessary ingredient that ensures the SU(2) commutation relations is the assignment of the phase factors which satisfies, for each pair of sites p,q,

$$e^{i\theta_{pq}}e^{-i\theta_{qp}} = -1. \tag{2}$$

One should notice that there is a large freedom in choosing phase factors satisfying condition (2). For instance, one could arbitrarily shift  $\theta_{pq} \rightarrow \theta_{pq} + 2k\pi$  with different integers k for each pair of lattice points p,q, or even perform an arbitrary simultaneous rotation for  $\theta_{pq}$  and  $\theta_{qp}$ . Standard plane angles  $-\pi < \theta \leqslant \pi$  measured from the x axis is just the simplest translation invariant choice on the flat infinite plane. It should be stressed that this large freedom does not alter the physical results, as long as all degrees of freedom are treated exactly. However, in any approximate treatment, this may introduce ambiguities that should be handled carefully, as we discuss below.

One salient feature of the JW transformation is that no constraint is needed on the new variables (cf., for instance, the Holstein-Primakoff or Schwinger bosons), but nonlocality is the main stumbling block in the approach.

The success of the JW transformation in one spatial dimension, in spite of being nonlocal, resides on the fact that XY nearest-neighbor (NN) interactions become local in fermion variables; this is not the case in two dimensions. Indeed, consider the XY Hamiltonian on a given 2D lattice,

$$H_{XY} = J \sum_{\langle p,q \rangle} (S_p^x S_q^x + S_p^y S_q^y), \tag{3}$$

where J is the exchange constant and the sum runs over all nearest neighbors  $\langle p,q \rangle$  on the lattice. In terms of fermion variables the Hamiltonian reads

$$H_{XY} = J \sum_{\langle p,q \rangle} \left( \frac{1}{2} c_p^{\dagger} e^{i\hat{\alpha}(p,q)} c_q + \text{H.c.} \right), \tag{4}$$

where

$$\hat{\alpha}(p,q) = \sum_{r}^{\prime} (\theta_{rq} - \theta_{rp}) c_{r}^{\dagger} c_{r}$$
 (5)

(the prime on the summation indicates that  $\theta_{rr}$  terms are absent). This phase is highly nonlocal; in the 1D case, the same expression becomes local due to the fact that the only two actual values for the angles are 0 and  $\pi$ . The nonlocality in 2D is usually overtaken by the introduction of an auxiliary gauge field  $A_{\mu}$ , which on the one hand represents the phases in Eq. (4) as the usual minimal coupling on the lattice, and on the other hand is governed by a Chern-Simons action. The Gauss law associated to the first-order Chern-Simons action imposes a constraint which in anyon language attaches half a quantum flux to each fermion, providing the statistical transmutation of fermions into bosons. Then, a mean-field treatment (known as average field approximation) of the gauge field can be done, leading in general to a quadratic NN interaction between fermions. However, the Chern-Simons

approach has serious difficulties when one deals with arbitrary lattice topologies (for example, the triangular lattice), and the associated mathematical problems are not yet solved.

We do not introduce such an auxiliary gauge field, but keep working with fermion variables. In order to perform numeric computations, one has to set a finite-size lattice and impose suitable boundary conditions. We use periodic boundary conditions, thus leading to a lattice on the torus. Moreover, the lattice size should be compatible with possible periodic configurations; in the case of a square lattice, size must be even in order not to interfere with the possible Néel order.

Now, it is not straightforward to define the JW transformation on the torus, 12 as the vector joining two different points is not unique. As one has to take care of condition (2), the vectors joining p with r and r with p must have arguments differing in  $\pi$ . We have to choose a unique segment joining each pair of points p,r, and then draw both vectors along it. One can choose this segment by a criterion of minimal distance. However, there exist pairs of points on the torus that can be joined by two or more different segments with minimal distance and hence an ad hoc criterion must be added. Any such criterion unavoidably breaks translation invariance, by preferring one segment over the rest. Naturally, we propose a criterion trying to minimize the violation of translation symmetry as follows: we set a principal finite-size lattice and extend it on a plane by periodicity; for each point on the principal lattice we consider also its periodic copies. Now, given a pair of sites, we look for the shortest segment joining either the points or their copies; when such a segment is unique, the procedure is translationally invariant. For those pair of points where one can find more than one minimal distance segment, we choose the one with both ends belonging to the principal lattice, thus breaking translation invariance. Finally, the angles  $\theta_{pr}$  and  $\theta_{rp}$  are computed as the arguments of the vectors joining p and r along the chosen segment. For convenience we also define that  $\theta_{nn}=0$ , in order to handle the restriction on the sums in Eqs. (1) and

As mentioned in the Introduction, the JW transformation is exact but the resulting Hamiltonian is highly nonlocal and some kind of approximation is necessary to proceed.

We propose here a variational approach to deal with the nonlocal phases in Eq. (4) and the quartic terms that can arise from  $S^z$  interactions. Working directly with fermion variables, we replace the local fermionic occupation numbers  $\hat{n}_p = c_p^{\dagger} c_p$  by their expectation values in an arbitrarily chosen variational state. This procedure leads to a multiparameter mean-field approach, which will in turn be evaluated self-consistently. This is the subject of the following section.

# III. VARIATIONAL APPROACH, APPLIED TO THE XXZ MODEL

To describe in full detail the method laid down above, we apply it to a generalized quantum spin- $\frac{1}{2}$  Heisenberg antiferromagnet in a square 2D periodic lattice, defined by the Hamiltonian

$$H_{XXZ} = J \sum_{\langle p,q \rangle} (S_{p}^{x} S_{q}^{x} + S_{p}^{y} S_{q}^{y} + \Delta S_{p}^{z} S_{q}^{z}) - h \sum_{p} S_{p}^{z}, \quad (6)$$

where  $\vec{S}_p = (S_p^x, S_p^y, S_p^z)$  represents the S = 1/2 spin operator at site p, J > 0 is the exchange constant, and  $0 < \Delta < \infty$  the "XXZ" anisotropy parameter. The first sum in Eq. (6) runs over all nearest neighbors in the given lattice, while the last term represents the interaction with a transverse external magnetic field h. We work on a periodic rectangular lattice of size  $K = N_x \times N_y$ .

Using the JW transformation defined in Eq. (1), the Hamiltonian can be written in terms of spinless fermions as

$$\begin{split} H_{XXZ} &= J \sum_{\langle p,q \rangle} \left[ \frac{1}{2} (c_p^{\dagger} e^{i\hat{\alpha}(p,q)} c_q + \text{H.c.}) + \Delta \left( c_p^{\dagger} c_p - \frac{1}{2} \right) \right. \\ &\times \left( c_q^{\dagger} c_q - \frac{1}{2} \right) \left] - h \sum_p \left( c_p^{\dagger} c_p - \frac{1}{2} \right), \end{split} \tag{7}$$

where the phase  $\hat{\alpha}(p,q)$  is defined in Eq. (5). Notice that the magnetic field h plays the rôle of a chemical potential for the JW fermions. In particular, we look for the ground state of the system (7) with fixed global magnetization M=0 (corresponding to h=0).

We implement a self-consistent mean-field solution by starting with a given fermion distribution profile  $\{n_p\}$  (which can be random or guided by some ansatz) on the lattice,

$$\langle \hat{n}_p \rangle = n_p \,, \tag{8}$$

which has to satisfy a global constraint to provide the given magnetization (here  $\sum n_p = K/2$  corresponds to M=0). We then replace the operator  $\hat{\alpha}(p,q)$  by its expectation value

$$\langle \hat{\alpha}(p,q) \rangle = \sum_{r} (\theta_{rq} - \theta_{rp}) n_r,$$
 (9)

where the angles  $\theta_{pq}$  are assigned following the criterion presented in the preceding section. To be precise, the principal lattice can be defined by indexing each site by a position pair (i,j), and setting the range  $i=0\cdots N_x-1$ ,  $j=0\cdots N_y-1$ . Periodic boundary conditions are then expressed by  $(i,j)\equiv (i+N_x,j)\equiv (i,j+N_y)$ .

Regarding the Ising term

$$S_{p}^{z}S_{a}^{z} = c_{p}^{\dagger}c_{p}c_{q}^{\dagger}c_{q} - \frac{1}{2}c_{p}^{\dagger}c_{p} - \frac{1}{2}c_{q}^{\dagger}c_{q} + \frac{1}{4}$$
 (10)

in Eq. (7), it is quartic in fermion operators, so it requires some mean-field approximation. In order to estimate the first term in Eq. (10) with a quadratic expression we propose the following:

$$c_p^{\dagger}c_p c_q^{\dagger}c_q \rightarrow \frac{1}{2}(c_p^{\dagger}c_p \langle c_q^{\dagger}c_q \rangle + c_q^{\dagger}c_q \langle c_p^{\dagger}c_p \rangle).$$
 (11)

This should be contrasted with a more standard proposal in the literature,  $c_p^{\dagger}c_pc_p^{\dagger}c_q \rightarrow c_p^{\dagger}c_p\langle c_q^{\dagger}c_q\rangle + c_q^{\dagger}c_q\langle c_p^{\dagger}c_p\rangle - \langle c_p^{\dagger}c_p\rangle\langle c_q^{\dagger}c_q\rangle$ . While there is no first-principles reason to distinguish both proposals, we wave chosen the one supported by best results in *a posteriori* evaluation of the g.s.

energy (see Sec. IV). Some other possibilities for handling the quartic term are discussed in Ref. 7.

At this step, the Hamiltonian can be written as

$$H_{XXZ}^{(MF)}(\{n_p\}) = \sum_{p,q} c_p^{\dagger} J_{pq}(\{n_p\}) c_q + C$$
 (12)

where

 $J_{na}$ 

$$= \begin{cases} \frac{J}{2}e^{i\langle\alpha(p,q)\rangle} & \text{if } \langle p,q\rangle \text{ nearest neighbors} \\ \frac{J\Delta}{2}\bigg(\sum_{neighbors\ r}\langle n_r\rangle - 4\bigg) & \text{if } p = q \\ 0 & \text{otherwise} \end{cases}$$

and  $C = KJ\Delta/2$ .

The main idea of the present paper is to provide a systematic way to compute an approximation to the true g.s. We first find the g.s. for the quadratic  $H_{XXZ}^{(MF)}(\{n_p\})$  by solving the one-particle (1P) spectrum and filling the system with the lowest-energy 1P states, up to the proper filling fixed by the total magnetization M. Then we compute from this approximate g.s. a new set of local densities  $n_p' = \langle \text{g.s.} | c_p^{\dagger} c_p | \text{g.s.} \rangle$ , which we use as a new input in Eq. (12) and iterate this procedure looking for a fixed point configuration for the density profile, i.e., a set of local densities  $\{n_p^*\}$  satisfying

$$n_p'(\{n_q^*\}) = n_p^*$$
 (14)

(13)

The existence of a fixed-point solution for this mapping and its eventual dependence on a given initial configuration is not at all obvious and has to be studied numerically.

In order to proceed with the method,  $H_{XXZ}^{(MF)}(\{n_p\})$  can be written in diagonal form

$$H_{XXZ}^{(MF)}(\{n_p\}) = \sum_{k=1}^{K} \epsilon(k) d_k^{\dagger} d_k + \text{const}, \qquad (15)$$

where  $\epsilon_k$  are the 1P eigenvalues of the quadratic part of  $H_{XXZ}^{(MF)}$ . Notice that k is just an integer index over the spectrum, not to be confused with the lattice momentum. Moreover, we order the eigenvalues ascendently.

The operators  $d_k$  are related to  $c_p$  by

$$d_k = \sum_p Q_{kp}^* c_p, \qquad (16)$$

where  $Q_{pk}$  is the matrix of eigenvectors of  $J_{pq}$ . We compute both  $\epsilon_k$  and  $Q_{pk}$  numerically. Q being unitary, the set of  $d_k$  operators satisfy fermion commutation relations  $\{d_k, d_{k'}^{\dagger}\}$  =  $\delta_{kk'}$ . Moreover, the total fermion number operator satisfies

$$N = \sum_{p=1}^{K} c_{p}^{\dagger} c_{p} = \sum_{k=1}^{K} d_{k}^{\dagger} d_{k}, \qquad (17)$$

making it easy to control the filling in terms of the new fermions.

We now construct the approximation to the quantum g.s. as the half-filled state that minimizes the energy, namely,

$$|g.s.\rangle = \prod_{k=1}^{K/2} d_k^{\dagger} |0\rangle. \tag{18}$$

Notice that this is a well-defined quantum state of K/2 particles, except for casual degeneracy of the 1P spectrum at the Fermi level. This is not the case for the XXZ model on the square lattice (see details below).

From  $|g.s.\rangle$  it is now easy to compute the approximate g.s. energy, as

$$E_{g.s.} = \langle g.s. | H_{XXZ}^{(MF)} | g.s. \rangle = \sum_{k < K/2} \epsilon_k + C.$$
 (19)

Also the local occupation numbers can be computed in this approximate g.s. as

$$n_p' = \langle g.s. | c_p^{\dagger} c_p | g.s. \rangle = \sum_{k \le K/2} Q_{pk}^* Q_{pk}.$$
 (20)

With these occupation numbers we start again the procedure: compute  $J_{pq}$  in MF, diagonalize the new  $H_{XXZ}^{(MF)}$ , etc.

We have found after thorough numerical investigations that a fixed-point solution for Eq. (14) always exists, but metastable solutions can also appear, depending on the initial configuration one chooses. In any case, one can distinguish metastable solutions from the best g.s. approximation simply by comparing their energies. Moreover, we describe below how this drawback can be naturally solved by introducing a thermal bath to kick the system out from the vicinity of metastable states.

Indeed, one can consider the effects of finite temperature by replacing the proposed ground state (18) by a thermal state  $|\Psi_{\beta}\rangle$ , compatible with the Fermi-Dirac 1P energy distribution at a given temperature,

$$n(\epsilon) = \frac{1}{1 + \exp[\beta(\epsilon - \overline{\epsilon})]},$$
 (21)

where  $\overline{\epsilon}$  is the 1P Fermi energy at half filling and  $\beta = 1/kT$  is the inverse temperature. In detail, this thermal state  $|\Psi_{\beta}\rangle$  is constructed as

$$|\Psi_{\beta}\rangle = \prod_{k \in \sigma} d_k^{\dagger} |0\rangle, \tag{22}$$

where  $\sigma$  is a set of K/2 1P states chosen with probability  $n(\epsilon(k))$  from some random simulation.

An exploration of the Hilbert space of the system by constructing a thermal state from a starting fermion distribution, computing from it the new local fermion distribution and again constructing a thermal state should be considered as a thermalization at the given temperature. It provides a source of thermal noise that has proven to help the system in finding lower-energy fixed points.

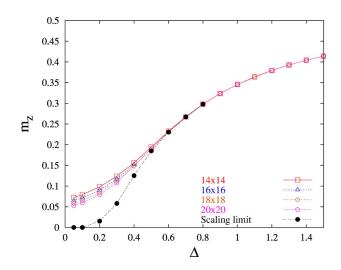


FIG. 1. Néel order parameter at fixed points as function of the anisotropy  $\Delta$ . Several lattice sizes and the scaling limit are shown.

The thermalization can be done through several steps at a given temperature, and then quenching to the pure quantum regime (T=0), or it can be implemented by gradually lowering T (annealing).

Besides, results at finite T can also be achieved by constructing a statistical ensemble of microscopic states compatible with T. Observables should then be computed as averages over the statistical ensemble. We do not attempt to complete this program in the present paper.

### IV. RESULTS

We have tested the iterative approach described in the preceding section with the well-known anisotropic XXZ model on periodic 2D square lattices of size up to  $20\times20$  sites, at zero total magnetization. The sizes of the lattice that we explored are by no means an upper limit, as our computations were made on a modest computer. The anisotropy parameter  $\Delta$  has been explored in a range from 0.05 to 1.5, including the isotropic SU(2) case ( $\Delta=1$ , Heisenberg model). As starting configurations  $\{n_p\}$  we have used random, uniform, and different amplitude staggered distributions. We performed several iterations and analyzed the evolution of the local fermion profile and the approximate g.s. energy. We report the results in terms of spin variables, noting that the local fermion occupation represents the local magnetization as  $m_z(p) = n_p - \frac{1}{2}$ .

Working at T=0, we have found that in general, from different starting configurations, the system rapidly finds a Néel order as stable ground-state approximation, after 15–20 iterations. The Néel order parameter, usually defined as the staggered or sublattice magnetization  $m_z$ , depends on the anisotropy parameter  $\Delta$ . Fluctuations around this staggered magnetization are typically of order  $10^{-8}$ . In Fig. 1 we plot the Néel order parameter  $m_z$  of the fixed-point solution for different values of  $\Delta$ , for several lattice sizes. Finite-size effects are noticeable for lower values of  $\Delta$ , so we also show the results of a finite-size scaling  $m_z(\infty)$  of our data, fitted with a power law  $m_z(K) = m_z(\infty) + c/K^{\alpha}$ . The corresponding

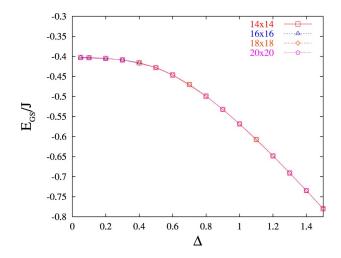


FIG. 2. g.s. energy as a function of the anisotropy  $\Delta$ . Data correspond to configurations plotted in Fig. 1.

g.s. energies per site are shown in Fig. 2 where one observes that scaling with the system size is clearly less important. We have observed that the 1P spectrum of the mean-field Hamiltonian (12) presents a gap  $2m_zJ\Delta$  for Néel ordered configurations, at the half-filling Fermi level. This is in agreement with Ref. 5 and makes the construction of  $|g.s.\rangle$  in Eq. (18) unambiguous. Limiting cases for the anisotropy have also been considered: the XY model ( $\Delta=0$ ) presents uniform filling ( $m_z=0$ ), with ground-state energy per site  $E_{g.s.}=-0.403J$ , while the Ising model ( $\Delta\to\infty$ ) presents full filling of one sublattice ( $m_z=0.5$ ) and energy  $E_{g.s.}=-0.5\Delta J$ . Had we used the more standard MF proposal for the Ising term, commented on after Eq. (11), we would have got higher g.s. energies for the whole range of  $\Delta$ .

In the case of random initial distributions, metastable configurations can show up; a detailed inspection of the local magnetization in these cases reveals the formation of antiferromagnetic domains, that is, the presence of the two possible Néel configurations in different regions. In Fig. 3 we show an example of such domains, at two different stages of a sample evolution. It is natural to expect that larger lattices favor the formation of these domains, as it indeed is observed. These configurations have higher energy than the uniform Néel state and correspond then to metastable configurations; correspondingly, they are not presented in Figs. 1 and 2.

When a thermal bath is simulated on random initial configurations, we have observed that metastable configurations are less likely to appear. After thermalization we let the system to cool down by either quenching or annealing as described in Sec. III, and complete the iterations at T=0. In fact, a few steps ( $\sim 10$ ) of thermalization with sufficiently high T completely avoid domain formation and lead to a unique fixed-point mean-field configuration; the required temperature is higher for larger lattices, being of the order of J for the lattice of  $20\times 20$ . We have checked that under general circumstances, quenching provides the fastest convergence method to the minimum-energy state. An example of the evolution of the Néel order parameter from an initial

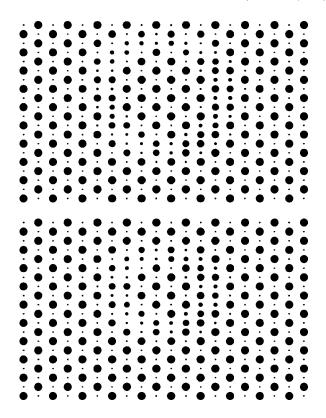


FIG. 3. Occupation patterns for a metastable configuration, where antiferromagnetic domains appear. The size of the points is proportional to the local fermion occupation number. These configurations occurred on a  $20\times20$  lattice, with  $\Delta=1.1$ , after ten steps of thermalization at T=0.2J, and 10 (upper panel) or 20 (lower panel) more steps of g.s. search at T=0. The smaller domain is seen to decrease in size under the simulated evolution.

random configuration, under thermalization with different temperatures, is shown in Fig. 4.

The results of the present MF computation show all the features expected for the Heisenberg antiferromagnet on the square lattice. They are of course not comparable to accurate numerical techniques, <sup>13</sup> but are in qualitative agreement with results from previous studies. In particular, in the scaling limit we obtain no Néel order for small anisotropy  $\Delta$ , where the system presumably has XY order. We can estimate a critical value  $\Delta^* \approx 0.2$ , above which Néel order develops. For the isotropic Heisenberg point  $\Delta = 1$  we obtain a sublattice magnetization  $m_z = 0.3453$ , with ground-state energy per site  $E_{\alpha s}/K = -0.5683J$ , to be compared, for instance, with corresponding quantum Monte Carlo values of 0.307 and -0.6694J. <sup>14</sup> One can compare also with MF descriptions of the usual statistical gauge field, which depending on the symmetry ansatz give magnetizations ranging from 0.39 to 0.44 and ground-state energies ranging from -0.48J to  $-0.648J.^{5,6}$ 

We must stress that our MF results are obtained with no *a priori* assumption on any kind of order. They thus provide at least an educated ansatz that could be refined by analytical adjustment of the relevant parameters and by the inclusion of fluctuations.

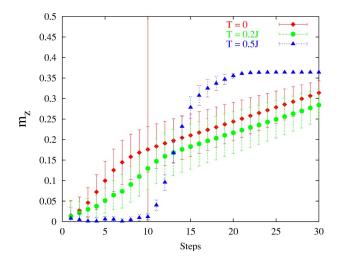


FIG. 4. Example of the evolution of the Néel order parameter from a sample initial random configuration. Data corresponds to the system depicted in Fig. 3, with a vertical line separating the thermal evolution and the  $T\!=\!0$  evolution. Error bars indicate the standard deviation of local magnetization from Néel order (reduced by a factor of 5 for clarity). Insufficient thermalization can lead to metastable configurations or to very slow convergence, while higher temperature dramatically improves convergence towards an ordered configuration.

# V. CONCLUSIONS

We have presented a self-consistent MF procedure for exploring the quantum ground state of any S=1/2 spin system on a 2D lattice. When tested on the XXZ model on a square lattice, the method provides the correct qualitative description of the system, with no *a priori* ansatz for any kind of order. We computed the values for the sublattice magnetization and g.s. energy for a wide range of values of the anisotropy parameter, which compare qualitatively well with the available numerical data, at least for  $\Delta=1$  where most accu-

rate data are available. Moreover, we have found that the sublattice magnetization as a function of the *XXZ* anisotropy shows the correct qualitative behavior, expected from a spinwave analysis.<sup>5</sup>

The present approach has a more general scope than previous MF computations, in the sense that it can be applied to *any* lattice topology, irrespective of the appearance of frustrating units, a fact that prevents the applicability of one of the most powerful numerical techniques such as quantum Monte Carlo. A magnetic field can be trivially added as a chemical potential for the JW fermions and hence magnetization curves could be obtained. Since the method is not based on any periodicity of couplings, it can be well suited to study disordered quantum spin systems, at the only price of increasing the CPU time. Last but not the least, the approach is naturally well suited for the study of the thermodynamics of these systems, since temperature can be added in a simple way.

Among other situations, it would be interesting to apply this technique to the Heisenberg quantum antiferromagnetic on the triangular lattice, where there is disagreement between Chern-Simons MF predictions<sup>8</sup> and numerical data about a magnetization plateaux at zero magnetization. Another case of interest is the kagomé lattice, where a quantum spin liquid is believed to be realized<sup>15</sup> (see also Ref. 16). This issue will be investigated elsewhere.

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