

Quantum compass model on the square lattice

Julien Dorier,¹ Federico Becca,² and Frédéric Mila¹

¹*Institut de Théorie des Phénomènes Physiques, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland*

²*INFN-Democritos, National Simulation Centre,*

and International School for Advanced Studies (SISSA), I-34014 Trieste, Italy

(Received 28 January 2005; revised manuscript received 27 May 2005; published 22 July 2005)

Using exact diagonalizations, Green's function Monte Carlo simulations and high-order perturbation theory, we study the low-energy properties of the two-dimensional spin-1/2 compass model on the square lattice defined by the Hamiltonian $H = -\sum_r (J_x \sigma_r^x \sigma_{r+e_x}^x + J_z \sigma_r^z \sigma_{r+e_z}^z)$. When $J_x \neq J_z$, we show that, on clusters of dimension $L \times L$, the low-energy spectrum consists of 2^L states which collapse onto each other exponentially fast with L , a conclusion that remains true arbitrarily close to $J_x = J_z$. At that point, we show that an even larger number of states collapse exponentially fast with L onto the ground state, and we present numerical evidence that this number is precisely 2×2^L . We also extend the symmetry analysis of the model to arbitrary spins and show that the twofold degeneracy of all eigenstates remains true for arbitrary half-integer spins but does not apply to integer spins, in which cases the eigenstates are generically nondegenerate, a result confirmed by exact diagonalizations in the spin-1 case. Implications for Mott insulators and Josephson junction arrays are briefly discussed.

DOI: 10.1103/PhysRevB.72.024448

PACS number(s): 75.30.Ds, 71.27.+a, 03.67.Lx

I. INTRODUCTION

Building on the deep understanding of the Heisenberg and other models of magnetism, it is a very common practice to describe discrete degrees of freedom as pseudospins, with the hope to gain insight from the form of the resulting magnetic model. A well-known example of considerable current interest shows up in the context of Mott insulators with orbital degeneracy: In an octahedral environment, the degeneracy of the d electrons is only partially lifted, and the remaining orbital degree of freedom is often described as a spin-1/2 or spin-1 for e_g and t_{2g} electrons, respectively.^{1,2} However, the situation is in general less simple than one might hope. Indeed, as already emphasized by Kugel and Khomskii, the symmetry of pseudospin Hamiltonians is in general much lower than SU(2), and there are cases where the properties of the resulting model are poorly understood. This is in particular the case in models where the anisotropy of the coupling in spin space is related to the orientation of the bond in real space. The simplest version of such a model on the square lattice is defined by the Hamiltonian

$$H = -J \sum_r (\tau_r^x \tau_{r+e_x}^x + \tau_r^z \tau_{r+e_z}^z), \quad (1)$$

where τ_r^α are the x and z components of a pseudospin operator. By analogy with the dipolar coupling between compass needles, this model has been called the compass model by Kugel and Khomskii.² Realistic models of orbital degeneracy are usually more complicated in several respects. In particular, the spins and pseudospins are usually coupled. Pure orbital models can be of direct relevance, however, if the spins order ferromagnetically or if the interaction between orbitals is much stronger than the interaction between the spins, as recently argued by Mostovoy and Khomskii in the context of NaNiO_2 .³ The precise symmetry is also usually more complicated than the simple case of this Hamiltonian, but we will

nevertheless concentrate on that model, considering it as a minimal model rather than a realistic one.

Interestingly, such models have appeared in other contexts as well. First, even in Mott insulators without orbital degeneracy, extra degrees of freedom can appear if the system is frustrated and, for instance, consists of spin-1/2 coupled triangles, like in the trimerized kagome lattice, in which case the chirality that keeps track of the extra degeneracy of each triangle plays a role similar to that of orbitals.⁴ In a magnetic field, this model has been predicted to exhibit a magnetization plateau at 1/3,⁵ and the low-energy properties inside the plateau can be described by a kind of compass model.⁶

More recently, the model of Eq. (1) with anisotropic couplings along the x and z directions has been proposed by Douçot and collaborators in the context of Josephson junction arrays.⁷

Despite its deceptive simplicity, the model of Eq. (1) is a formidable challenge, in many respects comparable to very frustrated magnets. To see this, let us follow Ref. 8 and consider the classical version of the model, in which spins are considered as classical vectors. In that case, as shown by Nussinov *et al.*, the ground state is highly degenerate, as in very frustrated magnets. First of all, all ferromagnetic states are degenerate, regardless of the relative orientation of the spins with respect to the lattice, as can be easily checked from Eq. (1). In addition, from any ferromagnetic state, one can construct other states by flipping all spins of a z column with respect to an x mirror, or equivalently by flipping all spins of an x line with respect to a z mirror. Since all these operations can be performed simultaneously and in any order, they generate a discrete degeneracy of order 2^{2L} in general, and 2^L if the spins are parallel to the x or z direction.

The effects of thermal fluctuations on the classical model have been convincingly identified by analytical and numerical approaches. Nussinov *et al.* have shown that an order-by-disorder mechanism is expected to lift the rotational degeneracy and to select states in which the spins point along the x

or z axis, leading to a nematic ground state since lines or columns of spins are still free to flip. Using extensive Monte Carlo simulations, Mishra *et al.* have shown that the two possible orientations along x or z lead to an effective Ising order parameter, and that the model undergoes a finite temperature phase transition of the Ising type.⁹

On the other hand, the understanding of the spin-1/2 version of the model is still preliminary. Most of the results have been obtained by Douçot *et al.*⁷ in their analysis of a generalized version of the model of Eq. (1) defined by the Hamiltonian

$$H = - \sum_r (J_x \tau_r^x \tau_{r+e_x}^x + J_z \tau_r^z \tau_{r+e_z}^z), \quad (2)$$

in which the couplings along the x and z directions can take different values. Using elegant symmetry arguments, Douçot *et al.* have shown that all eigenstates must be at least twofold degenerate. They have also shown that in the strongly asymmetric case ($J_x/J_z \ll 1$ or $J_z/J_x \ll 1$), the 2^L states that evolve adiabatically from the 2^L ground states of the decoupled Ising chain case ($J_x=0$ or $J_z=0$) should collapse onto each other. This perturbative argument does not apply close to $J_x=J_z$ though, and whether this remains true in the isotropic case could not be decided. Note that this is an important issue in the context of quantum bits in which they came across this model since the presence of a gap would help to protect the q -bits. More recently, Nussinov and Fradkin¹⁰ have shown that these models are dual to models of $p+ip$ superconducting arrays, and have discussed general properties of order parameters and phase transitions.

In this paper, we concentrate on the zero-temperature properties of the quantum version of the model. We start by a semiclassical analysis of the model of Eq. (1) and show that, as in many frustrated magnets, quantum fluctuations essentially have the same effect as thermal fluctuations regarding the lifting of classical degeneracy (Sec. II). We then turn to an extensive analysis of the model of Eq. (2) in the spin-1/2 case. As we shall see, there is no minus sign problem in the Green's function implementation of quantum Monte Carlo, which allows one to study the ground-state properties of very large clusters, i.e., up to 16×16 . Combined with the large number of symmetries, hence of different symmetry sectors that can be studied independently, this allowed us to reach definite conclusions regarding the low-energy spectrum, conclusions that agree with high-order perturbation theory. These results are presented in Sec. III. Finally, the symmetry analysis of Douçot *et al.* is extended to larger spins in Sec. IV, with the conclusion that integer and half-integer spins behave once more quite differently. Some implications of the present results are discussed in the last section of the paper.

II. SEMICLASSICAL COMPASS MODEL

In order to have a first insight into the properties of the quantum version of the compass model, we have performed a spin-wave analysis in the symmetric case defined by Eq. (1). In that respect, it is useful to emphasize that, as noticed in Refs. 8 and 9, the degeneracy is partly accidental and

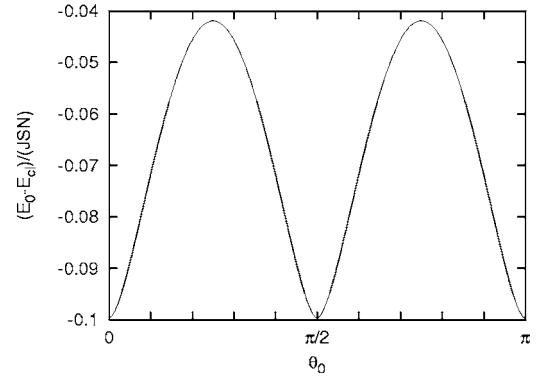


FIG. 1. Ground-state energy of the ferromagnetic states defined by $\mathbf{S}_r = S(\theta_0) = S \cos \theta_0 \mathbf{e}_x + S \sin \theta_0 \mathbf{e}_z$, including zero-point energy as a function of the angle θ_0 . $E_{cl} = -JNS^2$ is the classical ground-state energy and N is the number of sites.

partly due to symmetry. Indeed, in addition to the lattice translational symmetries, this model has two types of discrete symmetries: (i) The Q_i transformations, which flip the z component of all the spins of the column $r_x=i$, and the P_j transformations, which flip the x component of all spins of the line $r_z=j$. Note that the transformations Q_i (respectively P_j) could be seen as rotations of all the spins of the column (respectively line) about the \mathbf{e}_x axis (respectively \mathbf{e}_z) by an angle π . (ii) The simultaneous rotation $R_y(\pi/2)$ of all spins *and* of the lattice about an \mathbf{e}_y axis by an angle $\pi/2$. Starting from any state, these symmetries generate new states with exactly the same classical energy, and the degeneracy associated to these symmetries cannot be lifted by thermal fluctuations.⁹ However, the ground state also has an accidental degeneracy: All ferromagnetic states are degenerate regardless of the angle between the spins and the lattice. This degeneracy is not related to a symmetry since the model is not rotationally invariant. Accordingly, it has been found that the thermal fluctuations partially lift this degeneracy via an order-by-disorder mechanism, favoring the 2×2^L ground states with all spins parallel to \mathbf{e}_x or \mathbf{e}_z and implying a directional ordering of the spins. These favored states are the uniform state with all spins in the direction \mathbf{e}_x and all the states obtained by applying the symmetries $R_y(\pi/2)$, P_j , and Q_i . So, as anticipated, only the accidental degeneracy is lifted by thermal fluctuations.

The same idea applies to quantum fluctuations. Starting from an arbitrary ground state, one can bring it back into a ferromagnetic ground state applying only symmetry operations. But applying symmetry operations does not change the form of the Hamiltonian. The fluctuations around both states will thus have exactly the same form. Then it is sufficient to do the spin-wave expansion around the uniform classical ground states $\mathbf{S}_r = S \cos \theta_0 \mathbf{e}_x + S \sin \theta_0 \mathbf{e}_z$. To linear order in $1/S$, the energy can be brought into the form

$$H = E_0 + \frac{1}{2} \sum_q \omega_q(\theta_0), \quad (3)$$

with $\omega_q(\theta_0) = 4JS \sqrt{1 - \cos^2 \theta_0 \cos^2 k_x - \sin^2 \theta_0 \cos^2 k_z}$, and the resulting ground-state energy is plotted in Fig. 1. As in the

classical case with thermal fluctuations, the figure clearly shows that the angles $\theta_0=0, \pi/2, \pi, 3\pi/2$ are selected by quantum fluctuations since they minimize the energy. Applying the symmetries Q_i , P_j , and $R_y(\pi/2)$ to these states gives 2×2^L equivalent favored states, corresponding to 2^L states parallel to e_x and 2^L states parallel to e_z . So, as in the classical case, there is a directional ordering of the ground state.

As in many frustrated magnets like the J_1 - J_2 model on the square lattice for $J_2/J_1=1/2$, this calculation is not fully consistent since the correction to the magnetization diverges.¹¹ In the present case, the divergence comes from a line of zero energy along the $k_x=0$ direction when $\theta_0=0, \pi$ and along the $k_z=0$ direction when $\theta_0=\pi/2, 3\pi/2$. We have pushed the expansion to next order in $1/S$ and checked that a self-consistent mean-field decoupling of the four-boson terms suppresses the divergence.¹² At this approximation, the spectrum becomes gapped, which does not violate any general theorem since the model does not possess rotational symmetry, and long-range order is preserved even for spin-1/2.

In the anisotropic case ($J_x \neq J_z$), discrete rotational symmetry of the Hamiltonian as well as continuous rotational symmetry of the ground state are lost, leading to only the 2^L ground states with rows of parallel spins along the x axis for $J_x > J_z$ and columns of parallel spins along the z axis for $J_x < J_z$. Since these 2^L classical ground states are related by symmetries of the Hamiltonian, quantum fluctuations cannot lift this degeneracy.

III. QUANTUM COMPASS MODEL: SPIN-1/2

In this section, we turn to the spin-1/2 case for which we write the Hamiltonian

$$H = - \sum_r (J_x \sigma_r^x \sigma_{r+e_x}^x + J_z \sigma_r^z \sigma_{r+e_z}^z), \quad (4)$$

where σ_r^x and σ_r^z are Pauli matrices acting on the spin at site r . In the following, we will use the parametrization of the exchange integrals $J_x = J \cos \theta$ and $J_z = J \sin \theta$ with $\theta \in [0, \pi/2]$, and we will study the model on N -site square clusters of dimension $N=L \times L$.

Taking all symmetries into account, exact diagonalizations could be performed up to $L=5$. As we shall see, this is not sufficient to draw conclusions regarding the degeneracy of the ground state in the thermodynamic limit close to $J_x = J_z$. However, this model has the very interesting property that all nondiagonal matrix elements are negative. This has allowed us to implement the Green's function Monte Carlo algorithm,¹³ which gives access to the ground-state energy in a given symmetry sector, and to reach clusters up to $L=16$. Besides, one can choose quantum numbers so that all relevant low-energy states are ground states of a given symmetry sector. To see how this works, let us look more closely at the symmetries of the model.

In addition to the lattice translation symmetries, the Hamiltonian (4) has another type of discrete symmetries. The first one corresponds to the operators $Q_i = \prod_j \sigma_{i,j}^x$, which are the products of the σ_r^x on one column ($r_x=i$). These operations correspond to a rotation by an angle π about the e_x axis

of all the spins of a given column: $Q_i^{-1} \sigma_{i,j}^{y,z} Q_i = -\sigma_{i,j}^{y,z}$ and $Q_i^{-1} \sigma_{i,j}^x Q_i = \sigma_{i,j}^x$. The second one corresponds to the operators $P_j = \prod_i \sigma_{i,j}^z$, which are the products of the σ_r^z on one line ($r_z=j$), and which correspond to a rotation by an angle π about the e_z axis of all the spins of a given line: $P_j^{-1} \sigma_{i,j}^{x,y} P_j = -\sigma_{i,j}^{x,y}$ and $P_j^{-1} \sigma_{i,j}^z P_j = \sigma_{i,j}^z$. In the isotropic limit $J_x = J_z$, there is one more discrete symmetry: the global rotation $R_y(\pi/2)$ of all spins and lattice about the e_y axis by an angle $\pi/2$.

As emphasized by Douçot *et al.*, the P_j 's commute with each other, as well as the Q_i 's, but $[Q_i, P_j] \neq 0 \forall i, j$. This has two remarkable consequences: First, all eigenstates must be twofold degenerate. Besides, we can choose either the P_j 's or the Q_i 's to define symmetry sectors in which the Hamiltonian can be independently diagonalized. Since $P_j^2 = 1$ and $P_j^\dagger = P_j$, the eigenvalues of P_j are $p_j = \pm 1$, the same being true for the Q_i 's. Thus the Hamiltonian can be diagonalized in the symmetry sectors characterized by the set $(p_1, \dots, p_L), p_i = \pm 1$, or alternatively in the sectors defined by the eigenvalues of Q_i and characterized by the set $(q_1, \dots, q_L), q_i = \pm 1$.

To see how this works, let us start from the trivial case $J_x=0$. The model then consists of a set of decoupled Ising columns with eigenstates $|\mathbf{m}\rangle = |m_{1,1}\rangle \otimes |m_{1,2}\rangle \otimes \dots \otimes |m_{L,L}\rangle$, where $m_{i,j} = \pm 1$ is the eigenvalue of $\sigma_{i,j}^z$. The ground-state manifold contains 2^L states defined by $m_{i,1} = \dots = m_{i,L} = \pm 1$ and $i=1, \dots, L$. Clearly, all $|\mathbf{m}\rangle$ state are eigenstates of the P_j 's. Now, in any of the ground states, all p_j 's are equal since all lines are identical, and the ground-states manifold consists of 2^{L-1} states in the sector $p_1 = \dots = p_L = +1$ and 2^{L-1} states in the sector $p_1 = \dots = p_L = -1$.

The classification according to the Q_i 's is quite different. First, note that the states $\{|\mathbf{m}\rangle\}$ are not eigenstates of Q_i . However, if we denote by $|\uparrow\rangle_i$ (respectively $|\downarrow\rangle_i$) the ground state of column i with all the spins up (respectively down), then one can define two new ground states by $|+\rangle_i = (1/\sqrt{2})(|\uparrow\rangle_i + |\downarrow\rangle_i)$ and $|-\rangle_i = (1/\sqrt{2})(|\uparrow\rangle_i - |\downarrow\rangle_i)$. These new states are eigenstates of Q_i with eigenvalues ± 1 , respectively. So q_i can be either -1 or $+1$ for each column independently, and the ground-state manifold has one member in each of the 2^L sectors $(q_1, \dots, q_L), q_i = \pm 1$.

The case $J_z=0$ is connected to the case $J_x=0$ by the rotation $R_y(\pi/2)$. Since $R_y(\pi/2)^{-1} P_j R_y(\pi/2) = (-1)^L Q_{L-j}$ and $R_y(\pi/2)^{-1} Q_i R_y(\pi/2) = P_i$, the symmetry sectors are interchanged. So the ground state is made up of 2^L states in each 2^L sectors $(p_1, \dots, p_L) = (\pm 1, \dots, \pm 1)$.

So, as mentioned earlier, to determine the structure of the low-energy spectrum when going away from $J_x=0$ or $J_z=0$, it is always possible to choose the quantum numbers so that each state is the ground state of a given symmetry sector.

A. Exact diagonalization

The spectrum of the Hamiltonian (4) versus the asymmetry parameter θ has been determined for $L=2, 3, 4$, and 5 using exact diagonalization. Figure 2 presents the low-energy levels for $L=4$ and $L=5$. As expected, when $J_x, J_z \neq 0$, the ground state is twofold degenerate with one state in the sector $p_1 = \dots = p_L = +1$ and the other in the sector $p_1 = \dots = p_L = -1$. For $0 < J_z < J_x$, the 2^L -fold degeneracy of the ground

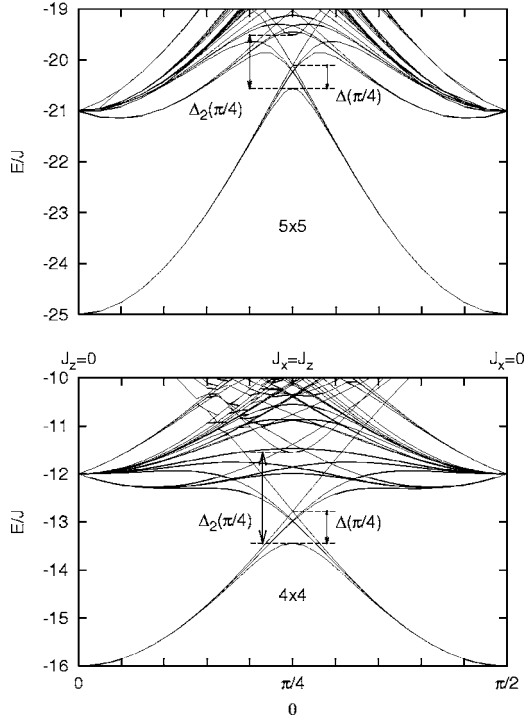


FIG. 2. Energy of the low-lying states vs anisotropy parameter θ for 4×4 and 5×5 lattices obtained by exact diagonalization ($J_x = J \cos \theta$; $J_z = J \sin \theta$).

state at $\theta=0$ (i.e., $J_z=0$) is lifted by the J_z term of the Hamiltonian. The lowest of these states is in the sector $p_1 = \dots = p_L = \pm 1$ and the highest in the sector $p_i = \pm (-1)^i$. The gap between these two states is denoted by $\Delta(\theta)$. As we will see in the following, $\Delta(\theta)$ goes to zero for all θ in the thermodynamic limit.

In the symmetric case $\theta = \pi/4$ (i.e., $J_x = J_z$), the adiabatic continuation of the degenerate ground states of the $J_x=0$ and $J_z=0$ cases generates only $2 \times 2^L - 2$ states, and not 2×2^L as one might naively expect from the semiclassical case. The reason is that the lowest pair of states is common to the two families of states coming from $J_x=0$ and $J_z=0$, while all other states cross at $J_x = J_z$ (see Fig. 2). This does not mean however that the low-energy sector has only $2 \times 2^L - 2$ states for very large systems. In fact, another pair of states is decreasing quite fast toward the ground state as a function of the size. Since these states correspond to the first twofold degenerate excited state of the sectors $p_1 = \dots = p_L = 1$ and $p_1 = \dots = p_L = -1$, one can keep track of their energy for all sizes. The gap between the ground state and these states, denoted by Δ_2 , is plotted in Fig. 3 as a function of $1/N$. These results are indeed consistent with a vanishing of this gap in the thermodynamic limit.¹⁴

B. Perturbation theory

Before discussing the results obtained for large clusters with Green's function quantum Monte Carlo, let us see what perturbation theory predicts regarding the scaling of the gap Δ in the limit $J_z \ll J_x$. To this purpose, the Hamiltonian is written as

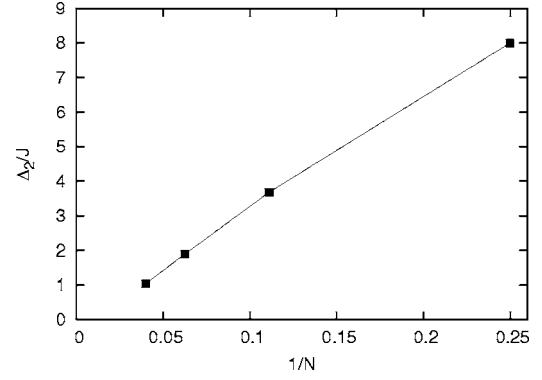


FIG. 3. Gap Δ_2 (see text) as a function of the number of sites N .

$$H = H_0 + V, \quad (5)$$

where $H_0 = -J_x \sum_r \sigma_r^x \sigma_{r+e_x}^x$ and $V = -J_z \sum_r \sigma_r^z \sigma_{r+e_z}^z$.

Since each term of V flips a pair of spins on neighboring chains, it is necessary to apply the perturbation at least L times on an $L \times L$ lattice to flip all spins of a pair of neighboring chains and reach another ground state. So the gap is expected to scale as $\Delta/J_x = a(bJ_z/J_x)^L$. One can be more precise though and determine the constants a and b from high-order perturbation theory. To first significant order in J_z/J_x , the gap Δ is given by the gap between lower and higher eigenvalues of the effective Hamiltonian

$$H_{\text{eff}}^{(L)} = \sum_{\nu_1 > 0} \dots \sum_{\nu_{L-1} > 0} \frac{P_0 V P_{\nu_1} V \dots V P_{\nu_{L-1}} V P_0}{(E_0 - E_{\nu_1}) \dots (E_0 - E_{\nu_{L-1}})}, \quad (6)$$

where P_ν is the projector on the ν th eigenspace of H_0 . This eigenspace has an energy $E_\nu = -J_x N + 4\nu J_x$, where ν can take the values $\nu = 0, 1, \dots, L/2$ when L is even and $\nu = 0, 1, \dots, (L-1)/2$ when L is odd. Let $\{|\nu, k\rangle : k = 0, 1, \dots\}$ be a basis of the ν th eigenspace of H_0 . We have to evaluate

$$\begin{aligned} & \langle 0, l | V P_{\nu_1} V \dots V P_{\nu_{L-1}} V | 0, k \rangle \\ &= (-J_z)^L \sum_{i_1, j_1} \dots \sum_{i_L, j_L} \\ & \times \langle 0, l | \sigma_{i_1, j_1}^z \sigma_{i_1, j_1+1}^z P_{\nu_1} \dots P_{\nu_{L-1}} \sigma_{i_L, j_L}^z \sigma_{i_L, j_L+1}^z | 0, k \rangle. \end{aligned}$$

For $L > 2$, the only contribution to Δ arises when the σ product flips two neighboring lines with $r_z = j$ and $r_z = j+1$. It corresponds to $j_1 = \dots = j_L = j$ and $i_1 = p(1), \dots, i_L = p(L)$ with $p \in S_L$ and S_L the set of $L!$ permutations. The ground state $|0, k\rangle$ contains only ferromagnetic lines in the x or $-x$ direction. So, for $m < L$, the state $\sigma_{p(m+1), j}^z \sigma_{p(m+1), j+1}^z \dots \sigma_{p(L), j}^z \sigma_{p(L), j+1}^z | 0, k\rangle$ cannot be in the ground-state manifold of H_0 , but it must be in one of the

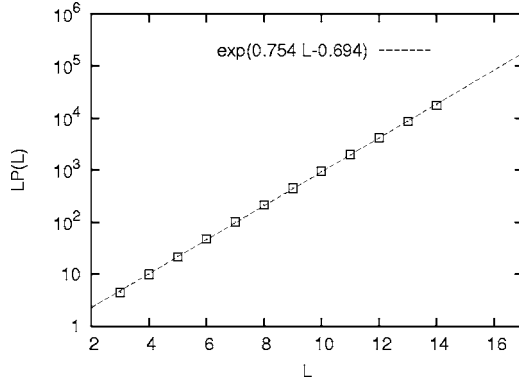


FIG. 4. Log-linear plot of $LP(L)$ vs the linear lattice size L . The squares are the results obtained numerically, and the dotted line is an exponential fit.

excited eigenspaces, say the $\nu_m(p)$ th. Then we can write

$$\begin{aligned} & \langle 0, l | VP_{\nu_1} V \cdots VP_{\nu_{L-1}} V | 0, k \rangle \\ &= (-J_z)^L \sum_{p \in S_n} \sum_j \\ & \times \langle 0, l | \sigma_{p(1),j}^z \sigma_{p(1),j+1}^z \cdots \sigma_{p(L),j}^z \sigma_{p(L),j+1}^z | 0, k \rangle \\ & \times \prod_{m=1}^{L-1} \delta_{\nu_m, \nu_m(p)}. \end{aligned}$$

Using $E_\nu = E_0 + 4\nu J_x$ and rearranging the σ^z 's, we get:

$$\begin{aligned} \langle 0, l | H_{\text{eff}}^{(L)} | 0, k \rangle &= - \frac{J_z^L}{(4J_x)^{L-1}} \sum_{p \in S_n} \frac{1}{\nu_1(p) \cdots \nu_{L-1}(p)} \\ & \times \langle 0, l | \sum_j \sigma_{1,j}^z \sigma_{1,j+1}^z \cdots \sigma_{L,j}^z \sigma_{L,j+1}^z | 0, k \rangle. \end{aligned}$$

Next, we note that, in terms of the pseudo spin $\tau_j^z = \sigma_{1,j}^z \cdots \sigma_{L,j}^z$, the operator $\sum_j \sigma_{1,j}^z \sigma_{1,j+1}^z \cdots \sigma_{L,j}^z \sigma_{L,j+1}^z$ is nothing but the Hamiltonian of the one-dimensional Ising model. So, the gap between the lowest and highest eigenvalues is $\lambda_{\max} - \lambda_{\min} = 2L$ when L is even and $\lambda_{\max} - \lambda_{\min} = 2(L-1)$ when L is odd. Finally, if we define $P(L)$ by

$$P(L) = \sum_{p \in S_n} \frac{1}{\nu_1(p) \cdots \nu_{L-1}(p)}, \quad (7)$$

the gap Δ becomes

$$\Delta/J_x = \begin{cases} 8LP(L)(J_z/4J_x)^L & \text{if } L \text{ is even,} \\ 8(L-1)P(L)(J_z/4J_x)^L & \text{if } L \text{ is odd.} \end{cases} \quad (8)$$

The dominant behavior of $P(L)$ has been determined numerically (see Fig. 4). It turns out that $LP(L) \approx \exp(0.754L - 0.694)$, which leads to:

$$\Delta/J_x = \begin{cases} 3.997(0.531J_z/J_x)^L & \text{if } L \text{ is even,} \\ 3.997(1 - 1/L)(0.531J_z/J_x)^L & \text{if } L \text{ is odd.} \end{cases} \quad (9)$$

It has the correct $(J_z/J_x)^L$ behavior which corresponds to the exact result for the two-line system.⁷ So, when $(J_z/J_x) \ll 1$, this approximation predicts $\Delta \rightarrow 0$ in the thermodynamic

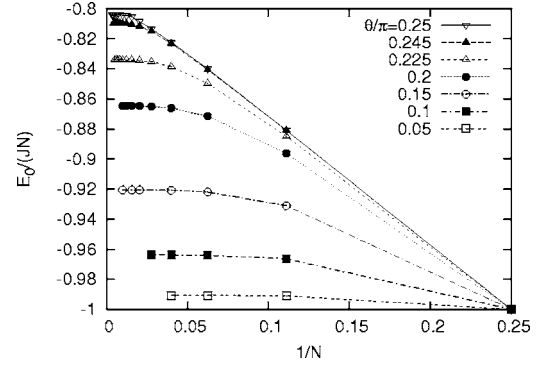


FIG. 5. Ground-state energy E_0 vs the number of sites N for various values of the asymmetry parameter θ .

limit. Moreover, since $0.531(J_z/J_x) < 1$ even for $J_z/J_x = 1$, it seems likely that this scaling will remain true up to the symmetric limit $J_x = J_z$. As we shall see, this is confirmed by the Green's function Monte Carlo results.

C. Green's function Monte Carlo

If the Hamiltonian of a model has only nonpositive off-diagonal matrix elements, which is the case here, the Green's function Monte Carlo method¹³ allows one to calculate the ground-state energy of a given symmetry sector by using a stochastic approach. The algorithm we have used is the implementation with a fixed number of walkers described in detail by Calandra and Sorella,¹³ and the guiding function is given by

$$|\psi_G\rangle = \exp\left(\frac{1}{2} \sum_{r,r'} v_{r,r'} \sigma_r^z \sigma_{r'}^z\right) |F_x\rangle, \quad (10)$$

where $|F_x\rangle$ is the ferromagnetic state in the x direction such that $\sigma_r^x |F_x\rangle = |F_x\rangle \forall r$. The parameters $v_{r,r'}$ were determined in order to minimize the energy of the guiding function. The ground-state energy has been determined in each sector (p_1, \dots, p_L) separately, which corresponds to the energy of the first 2^L states of the full Hilbert space (the states coming from the limit $J_z = 0$ ground state in Fig. 2), and gives access to the gap $\Delta(\theta)$.

Let us first discuss the scaling of the energy per site as a function of the system size. As can be seen in Fig. 5, the energy per site is strongly size-dependent up to a certain size (8×8 for $J_x = J_z$), and is very little size-dependent for larger clusters. This indicates that strong finite-size effects are to be expected, especially close to the symmetric point, justifying the use of quantum Monte Carlo to get information on large clusters.

Figure 6 shows a log-linear plot of the gap Δ versus the linear lattice size L for various values of the asymmetry parameter θ . Perturbation theory predicts that the scaling of Δ is given by a power law $\Delta/J_x \propto \alpha^L$, with $\alpha \approx 0.531J_z/J_x$. To check this prediction, we have fitted the results of Fig. 6 with a straight line for each value of θ , keeping only sizes beyond which the scaling is approximately linear. The values of α deduced from this fit are plotted in Fig. 7 as a function of J_z/J_x . Remarkably, the relation between α and J_z/J_x is quite

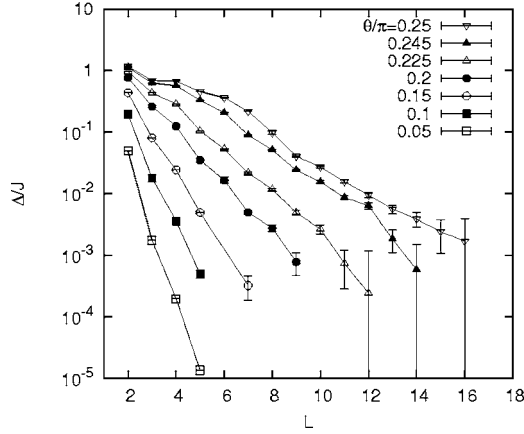


FIG. 6. Gap Δ vs linear lattice size L for various values of the anisotropy parameter θ . For $L=2, 3, 4, 5$ the results were obtained from exact diagonalization.

linear up to $J_x=J_z$, which seems to justify the perturbation theory in this limit. Moreover, a fit gives $\alpha \approx 0.55J_z/J_x$, in good agreement with the perturbation theory prediction $\alpha \approx 0.531J_z/J_x$. In fact, for small J_z/J_x , even the prefactor and the even-odd effect predicted by the perturbation theory agree with the results of Fig. 6. All these results lead us to the conclusion that the gap Δ indeed follows a power law $\Delta/J \sim \alpha^L$, with $\alpha < 1$ when $J_z \leq J_x$, implying that $\Delta \rightarrow 0$ in the thermodynamic limit. Thus the 2^L states coming from the limit $\theta=0$ ($J_z=0$) ground-state collapse in the thermodynamic limit, as long as $J_z \leq J_x$. Using the rotation $R_y(\pi/2)$, the same result holds true for the 2^L states coming from the limit $\theta=\pi/2$ (i.e., $J_x=0$) ground-state, as long as $J_z \geq J_x$. The conclusion is that there are 2^L states collapsing exponentially fast onto each other when $J_x \neq J_z$, and at least a $2 \times 2^{L-2}$ when $J_x=J_z$. As we argued above, the actual number is very probably actually equal to 2×2^L , in agreement with the semiclassical analysis.

D. The transition at $J_x=J_z$

From the previous analysis, it turns out that for $J_z > J_x$, the low-energy sector of the spectrum contains 2^L states, which

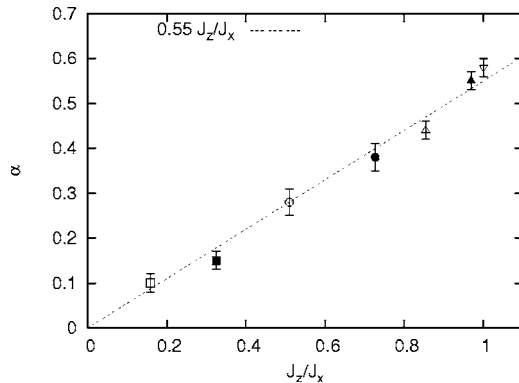


FIG. 7. α vs J_z/J_x , where α is the gap-scaling constant $\Delta \sim \alpha^L$. The symbols are the results obtained with Green's function Monte Carlo, and the dotted line is fitted to these values.

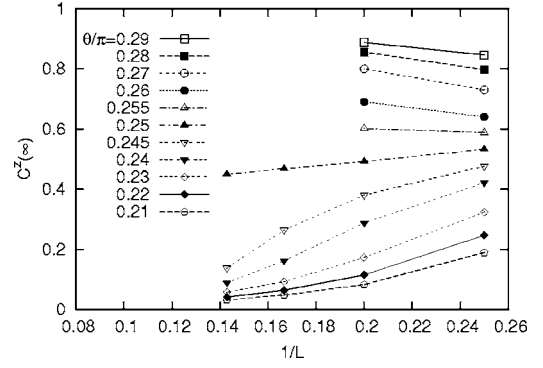


FIG. 8. Long-range correlations in the ground state along z direction $C^z(\infty)$ (see text) as a function of the linear lattice size L for various values of the anisotropy parameter θ .

consist of weakly coupled chains in the z direction and which are adiabatically connected to the ground-state manifold of the $J_x=0$ limit. For $J_z < J_x$, the low-energy sector of the spectrum also contains 2^L states, but this time they are adiabatically connected to the ground-state manifold of the $J_z=0$ limit. The open problem that demands a clarification is the nature of the evolution between these two different phases. In this regard, different scenarios are allowed. One possibility is that there is a smooth crossover between the two limiting cases without any critical behavior related to the isotropic point. On the other hand, another possibility is that $J_x=J_z$ is a true transition point, associated either to a first-order or to a second-order (or more generally to a continuous) transition.

In order to clarify this important issue, we calculate the ground-state static correlations $C^z(\mathbf{r}) = \langle \sigma_0^z \sigma_r^z \rangle$ between the z component of the spins at distance \mathbf{r} . This kind of correlation, which is diagonal in the Ising basis, can be easily calculated by using both exact diagonalizations and Green's function Monte Carlo. It turns out that $C^z(\mathbf{r})$ is nonzero only in the z direction and, therefore, we are only interested in $C^z(\mathbf{r}) \equiv C^z(r\mathbf{e}_z)$. In particular, to see if the system exhibits long-range order, we consider the long-distance behavior of $C^z(\mathbf{r})$, i.e., $C^z(\infty) = \lim_{r \rightarrow \infty} C^z(\mathbf{r})$, which can be extracted by fitting the correlations with an exponential form $C^z(\mathbf{r}) = a \exp(-b|r|) + C^z(\infty)$, suitable for this kind of model. In Fig. 8, we report $C^z(\infty)$ as a function of the linear lattice size L for various values of the anisotropy parameter θ . For $\theta > \pi/4$ ($J_z > J_x$), it is very hard to have a reliable estimate of the correlations within Green's function Monte Carlo, but the exact diagonalization results already provide clear evidence for a finite value of $C^z(\infty)$ in the thermodynamic limit, indicating the presence of a spin order in the z direction. On the other hand, for $\theta < \pi/4$ ($J_z < J_x$), reliable Green's function Monte Carlo estimates can be extracted for larger sizes, and $C^z(\infty)$ strongly decreases as the lattice size increases, a result consistent with a vanishing value in the thermodynamic limit. It should be emphasized that, for the correlations between the x component of the spins along the x direction, $C^x(\mathbf{r}) = \langle \sigma_0^x \sigma_r^x \rangle$ can be related to $C^z(\mathbf{r})$ by a mirror symmetry around $\theta = \pi/4$. Therefore, the long-range correlation along the x direction $C^x(\infty) = \lim_{r \rightarrow \infty} C^x(\mathbf{r})$ is expected to be zero

for $\theta > \pi/4$ ($J_z > J_x$) and finite for $\theta < \pi/4$ ($J_z < J_x$).

The most important result that comes out from this analysis is that the behavior of the correlation functions indicates that there is a first-order phase transition at $J_x = J_z$, with a sudden jump in $C^z(\infty)$ that passes from a finite value, $C^z(\infty) \sim 0.34$, for $J_z = J_x$ to zero for $J_z < J_x$ (see Fig. 8). Of course, our results cannot give a definite answer to this delicate issue, but, nonetheless, give a rather strong indication in favor of a noncontinuous transition at the isotropic point.

IV. GENERAL SPIN

The symmetry arguments used for spin-1/2 can be easily extended to arbitrary spins. Let us consider the system with N spins S on a $L \times L$ lattice described by the compass model Hamiltonian

$$H = - \sum_r \left(J_x S_r^x S_{r+e_x}^x + J_z S_r^z S_{r+e_z}^z \right). \quad (11)$$

It is straightforward to check that the generalizations of the P_j and Q_i defined by

$$P_j = \prod_l i e^{-i\pi S_{i,j}^z}, \quad (12)$$

$$Q_i = \prod_j i e^{-i\pi S_{i,j}^x}, \quad (13)$$

for integer spins and by

$$P_j = \prod_l e^{-i\pi S_{i,j}^z}, \quad (14)$$

$$Q_i = \prod_j e^{-i\pi S_{i,j}^x}, \quad (15)$$

for half-integer spins commute with the Hamiltonian. However, it is easy to check that the commutator $[Q_i, P_j]$ vanishes for integer spins, whereas it does *not* vanish for half-integer spins ($\{Q_i, P_j\} = 0$). Indeed, the only terms in the product which do not trivially commute are those on the site (i, j) . So we just have to show that $[e^{-i\pi S_{i,j}^x}, e^{-i\pi S_{i,j}^z}] = 0$ for integer spins and $\{e^{-i\pi S_{i,j}^x}, e^{-i\pi S_{i,j}^z}\} = 0$ for half-integer spins. The operator $e^{-i\pi S_{i,j}^z} = R_z(\pi)$ corresponds to the spin rotation by an angle π about the z axis acting at site (i, j) . Applying this rotation to $e^{-i\pi S_{i,j}^x}$ gives

$$\begin{aligned} R_z^{-1}(\pi) e^{-i\pi S_{i,j}^x} R_z(\pi) &= \sum_n \frac{(-i\pi)^n}{n!} R_z^{-1}(\pi) (S_{i,j}^x)^n R_z(\pi) \\ &= \sum_n \frac{(-i\pi)^n}{n!} (-S_{i,j}^z)^n = e^{i\pi S_{i,j}^z}. \end{aligned}$$

However for integer spins, $e^{i\pi S_{i,j}^z} = e^{-i\pi S_{i,j}^z}$, while for half-integer spins, $e^{i\pi S_{i,j}^z} = -e^{-i\pi S_{i,j}^z}$, which terminates the proof. This has two important consequences. First of all, in the argument of Douçot *et al.*, the fact that $[Q_i, P_j] \neq 0$ was crucial to show that each state was two fold degenerate. We thus

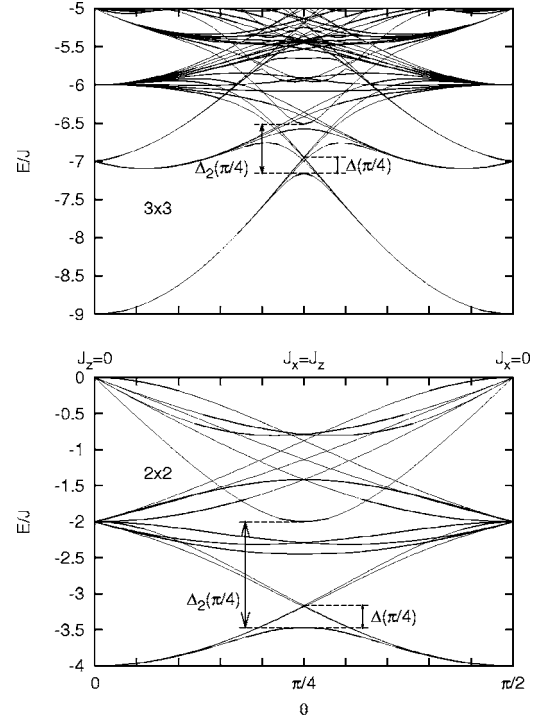


FIG. 9. Spectrum vs asymmetry parameter θ for linear lattice sizes $L=2$ and $L=3$ obtained by exact diagonalization ($J_x = J \cos \theta$ and $J_z = J \sin \theta$).

expect that for all integer spins, the eigenstates are generically nondegenerate. Besides, for integer spins, since all Q_i 's commute with all P_j 's, one can use all these symmetries simultaneously, leading to 2^{2L} different symmetry sectors.

We have checked these predictions for $S=1$ with exact diagonalizations of clusters of size $L=2$ and $L=3$ (see Fig. 9). Indeed, the ground state is nondegenerate for all $J_x, J_z \neq 0$, and it is in the only symmetry sector $p_1 = \dots = p_L = q_1 = \dots = q_L = (-1)^L$ connecting the ground states in the limits $J_x=0$ and $J_z=0$. The $J_z=0$ (respectively $J_x=0$) ground-state 2^L -fold degeneracy is partially lifted by the J_z (respectively J_x) term of the Hamiltonian, creating a gap Δ . As in the spin-1/2 model, the gap between the ground state and the first excited state which has the same degeneracy and is in the same symmetry sector as the ground state is denoted by Δ_2 . The gaps Δ and Δ_2 are smaller for $L=3$ than for $L=2$, and one can conjecture that these gaps go to zero in the thermodynamic limit. In this case, the ground state would have the same degeneracy as for spin-1/2. A definite conclusion would clearly require a study of larger clusters though.

V. CONCLUSION

Using a variety of approaches, we have obtained a coherent picture of the zero-temperature properties of the quantum compass model. On a finite cluster, we have confirmed that all eigenstates of the spin-1/2 model are at least twofold degenerate, a result that we have extended to arbitrary half-integer spins, while they are not necessarily degenerate for integer spins. However, the degeneracy that remains when thermal or semiclassical quantum fluctuations are introduced,

namely, the possibility to flip the spins along lines or columns, is still present as a manifold of states which collapse exponentially fast onto the ground state upon increasing the size of the lattice. This was already known to be the case for the asymmetric case not too close to $J_x = J_z$. Thanks to extensive quantum Monte Carlo simulations, we have shown that this remains true up to the symmetric case $J_x = J_z$, and that the number of these states (2^L when $J_x \neq J_z$, 2×2^L when $J_x = J_z$) agrees with the degeneracy predicted by the semiclassical analysis.

Physically, this has two consequences. Regarding orbital fluctuations in Mott insulators, in which case the symmetric version of the model ($J_x = J_z$) seems more appropriate, the present results suggest the absence of simple orbital long-range order for quantum spins in the thermodynamic limit even at zero temperature. Nevertheless, the system is expected to develop long-range correlations in one spatial direction, and, as in the case of thermal fluctuations for classical spins, the possibility to choose between the x and z directions should still lead to a finite-temperature Ising transition.

Regarding Josephson junction arrays, one of the important issues is to ensure that the twofold degenerate ground state is well protected by a gap to all excited states. As noticed by Douçot *et al.*, this requires working with not-too-large systems if a family of states collapse onto the ground state in the thermodynamic limit, as they already showed to be the case for $J_x \ll J_z$. Their results suggested however that there might be a quantum phase transition to a gapped phase around $J_x = J_z$ in which the gap to all excited states would remain finite even in the thermodynamic limit. This possibility is clearly ruled out by the present results.

ACKNOWLEDGMENTS

We thank Mike Ma for enlightening discussions about the symmetries of the model, Arnaud Ralko for useful discussions about Green's function Monte Carlo, and Benoît Douçot for a critical reading of the manuscript. This work was supported by the Swiss National Fund and by MaNEP. F.B. was supported by INFM and by (COFIN 2004).

¹K. I. Kugel and D. I. Khomskii, *Sov. Phys. Usp.* **25**, 231 (1982).

²K. I. Kugel and D. I. Khomskii, *Sov. Phys. JETP* **37**, 725 (1973).

³M. V. Mostovoy and D. I. Khomskii, *Phys. Rev. Lett.* **89**, 227203 (2002).

⁴F. Mila, *Phys. Rev. Lett.* **81**, 2356 (1998).

⁵K. Hida, *J. Phys. Soc. Jpn.* **70**, 3673 (2001); D. C. Cabra, M. D. Grynberg, P. C. W. Holdsworth, and P. Pujol, *Phys. Rev. B* **65**, 094418 (2002); J. Schulenburg, A. Honecker, J. Schnack, J. Richter, and H.-J. Schmidt, *Phys. Rev. Lett.* **88**, 167207 (2002); A. Honecker, J. Schulenburg, and J. Richter, *J. Phys.: Condens. Matter* **16**, S749 (2004).

⁶D. C. Cabra (private communication).

⁷B. Douçot, M. V. Feigel'man, L. B. Ioffe, and A. S. Iosevich, *Phys. Rev. B* **71**, 024505 (2005).

⁸Z. Nussinov, M. Biskup, L. Chayes, and J. van den Brink, *Euro-*

phys. Lett. **67**, 990 (2004).

⁹A. Mishra, M. Ma, F.-C. Zhang, S. Guertler, L.-H. Tang, and S. Wan, *Phys. Rev. Lett.* **93**, 207201 (2004).

¹⁰Z. Nussinov and E. Fradkin, *Phys. Rev. B* **71**, 195120 (2005).

¹¹P. Chandra and B. Douçot, *Phys. Rev. B* **38**, 9335 (1988).

¹²A similar calculation for a three-dimensional spin-orbital model, relevant to describe the physics of LaTiO₃, has been done by G. Khaliullin, *Phys. Rev. B* **64**, 212405 (2001).

¹³Nandini Trivedi and D. M. Ceperley, *Phys. Rev. B* **41**, 4552 (1990). In particular, we used the algorithm described by M. Calandra-Buonaura and S. Sorella, *Phys. Rev. B* **57**, 11446 (1998).

¹⁴Unfortunately, this state is not accessible to the quantum Monte Carlo algorithm, which only gives access to the ground-state energy of a given sector.