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Hidden dimer order in the quantum compass model

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We introduce an exact spin transformation that maps frustrated $Z_{i,j}Z_{i,j+1}$ and $X_{i,j}X_{i+1,j}$ spin interactions along the rows and columns of the quantum compass model (QCM) on an $L\times L$ square lattice to $(L-1)\times(L-1)$ quantum spin models with $2(L-1)$ classical spins. Using the symmetry properties we unravel the hidden dimer order in the QCM, with equal two-dimer correlations $\langle X_{i,i}X_{i+1,i}X_{k,l}X_{k+1,l}\rangle$ and $\langle X_{i,i}X_{i+1,i}X_{l,k}X_{l+1,k}\rangle$ in the ground state, which is independent of the actual interactions. This order coexists with Ising-type spin correlations which decay with distance.

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I. INTRODUCTION

The quantum compass model (QCM) originates from the frustrated (Kugel-Khomskii) superexchange[1] in transition-metal oxides with degenerate $3d$ orbitals. Recent interest in this model is motivated by its interdisciplinary character as it plays a role in the variety of phenomena beyond the correlated oxides. It describes a quantum phase transition between competing types of order when anisotropic interactions are varied through the isotropic point, as shown by an analytical method,[2] mean-field (MF),[3] and numerical studies.[4–8] The QCM is dual to the models of $p+ip$ superconducting arrays[9] and to the toric code model in a transverse field.[10] It was also suggested as an effective model for Josephson arrays of protected qubits,[2] as realized in recent experiment.[11] Finally, it could describe polar molecules in optical lattices and systems of trapped ions.[12]

In spite of several numerical studies,[4–8] the nature of spin order in the two-dimensional (2D) QCM is not yet fully understood. By an exact solution of the QCM on a ladder we have shown, however, that the invariant subspaces may be deduced using the symmetry.[13] The 2D QCM shows a self-duality[9] which might serve to reveal nontrivial hidden symmetries.[14] In this Rapid Communication we employ exact spin transformations which allow us to discover a surprising hidden dimer order in the QCM which manifest itself by exact relations between four-point correlation functions in the ground state. We also demonstrate nonlocal MF splitting of the QCM in the ground subspace and determine spatial decay of spin correlations in the thermodynamic limit.

II. REDUCED HAMILTONIAN

We consider the anisotropic ferromagnetic QCM for pseudospins 1/2 on an $L\times L$ square lattice with periodic boundary conditions (PBC)

$$\mathcal{H}(\alpha) = -\sum_{i,j=1}^{L}\{(1-\alpha)X_{i,j}X_{i+1,j} + \alpha Z_{i,j}Z_{i,j+1}\}, \tag{1}$$

where $\{X_{i,j},Z_{i,j}\}$ stand for Pauli matrices at site (i,j), i.e., $X_{i,j}\equiv\sigma^x_{i,j}$ and $Z_{i,j}\equiv\sigma^z_{i,j}$ components, interacting on vertical and horizontal bonds. In case of L being even, this model is equivalent to the antiferromagnetic QCM. We can easily construct a set of $2L$ operators which commute with the Hamiltonian but anticommute with one another:[2] $P_i\equiv\prod_{j=1}^{L}X_{i,j}$ and $Q_j\equiv\prod_{i=1}^{L}Z_{i,j}$. Below we will use as symmetry operations all $R_i\equiv P_iP_{i+1}$ and Q_j to reduce the Hilbert space; this approach led to the exact solution of the compass ladder.[13] The QCM, Eq. (1), can be written in common eigenbasis of $\{R_i,Q_j\}$ operators using

$$X_{i,j} = \prod_{p=i}^{L}\widetilde{X}_{p,j}, \quad \widetilde{X}_{i,j} = X'_{i,j-1}X'_{i,j}, \tag{2}$$

$$Z_{i,j} = \widetilde{Z}_{i-1,j}\widetilde{Z}_{i,j}, \quad \widetilde{Z}_{i,j} = \prod_{q=j}^{L}Z'_{i,q}, \tag{3}$$

where $\widetilde{Z}_{0,j}\equiv 1$ and $X'_{i,0}\equiv 1$. One finds that the transformed Hamiltonian, $\mathcal{H}'(\alpha)=-(1-\alpha)H'_x-\alpha H'_z$, contains no $\widetilde{X}_{L,j}$ and no $Z'_{i,L}$ operators so the corresponding $\widetilde{Z}_{L,j}$ and $X'_{i,L}$ can be replaced by their eigenvalues q_j and r_i, respectively. The Hamiltonian $\mathcal{H}'(\alpha)$ is dual to the QCM $\mathcal{H}(\alpha)$ of Eq. (1) in the thermodynamic limit; we give here an explicit form of its x part

$$H'_x = \sum_{i=1}^{L-1}\left\{\sum_{j=1}^{L-2}X'_{i,j}X'_{i,j+1} + X'_{i,1} + r_iX'_{i,L-1}\right\} + P'_1 + \sum_{j=1}^{L-2}P'_jP'_{j+1} + rP'_{L-1}, \tag{4}$$

where $r=\prod_{i=1}^{L-1}r_i$, and new nonlocal $P'_j=\prod_{p=1}^{L-1}X'_{p,j}$ operators originate from the PBC. The z part H'_z follows from H'_x by lattice transposition $X'_{i,j}\to Z'_{i,j}$, and by $r_i\to s_j=q_jq_{j+1}$. Ising variables r_i and s_j are the eigenvalues of the symmetry operators R_i and $S_j=Q_jQ_{j+1}$.

Instead of the initial $L\times L$ lattice of quantum spins, one finds here $(L-1)\times(L-1)$ internal quantum spins with $2(L-1)$ classical boundary spins. The missing spin is related to the Z_2 symmetry of the QCM and makes every energy level at least doubly degenerate. Although the form of Eq. (4) is complex, the size of the Hilbert space is reduced in a dramatic way by a factor 2^{2L-1} which makes it possible to perform easily exact (Lanczos) diagonalization of 2D $L\times L$ clusters up to $L=5$ $(L=6)$.

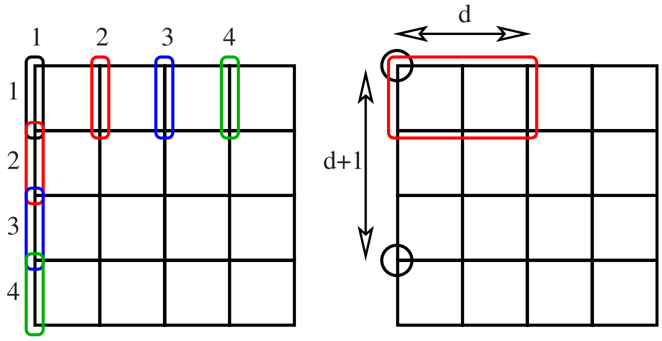

FIG. 1. (Color online) Example of the application of the proved identities in two cases: left panel—Eq. (10) for a chosen dimer $\mathcal{D}_{i,j} \equiv X_{i,j}X_{i+1,j}$ (label 1), correlations of $\mathcal{D}_{i,j}$ with a given $\mathcal{D}_{k,l}$ are the same for dimers $\mathcal{D}_{k,l}$ marked with the same label (color); right panel—Eq. (11) long-range correlation function $\langle X_{i,j}X_{i+d+1,j}\rangle$ along the column (circles) is equal to the $2d$—point $\langle XX,\ldots,X\rangle$ correlation function along the row (frame of length d).

III. EQUIVALENT SUBSPACES

The original QCM of Eq. (1) is invariant under the transformation $X' \leftrightarrow Z'$, if one also transforms the interactions, $\alpha \leftrightarrow (1-\alpha)$. This implies that subspaces $(\vec{r},\vec{s})$ and $(\vec{s},\vec{r})$ give the same energy spectrum which sets an equivalence relation between the subspaces—two subspaces are equivalent means that the QCM, Eq. (1), has in them the same energy spectrum. This relation becomes especially simple for $\alpha=\frac{1}{2}$ when for all r_i's and s_i's subspaces $(\vec{r},\vec{s})$ and $(\vec{s},\vec{r})$ are equivalent.

Now we will explore another important symmetry of the 2D compass model reducing the number of nonequivalent subspaces—the translational symmetry. We note from Eq. (4) that the reduced Hamiltonians are not translationally invariant for any choice of $(\vec{r},\vec{s})$ even though the original Hamiltonian is. This means that translational symmetry must impose some equivalence conditions among subspace labels $\{\vec{r},\vec{s}\}$. To derive them, let us focus on translation along the rows of the lattice by one lattice constant. Such translation does not affect the P_i symmetry operators because they consist of spin operators multiplied along the rows but changes Q_j into Q_{j+1} for all $j<L$ and $Q_L \rightarrow Q_1$. This implies that two subspaces $(\vec{r},q_1,q_2,\ldots,q_L)$ and $(\vec{r},q_L,q_1,q_2,\ldots,q_{L-1})$ are equivalent for all values of $\vec{r}$ and $\vec{q}$. Now this result must be translated into the language of $(\vec{r},\vec{s})$ labels with $s_j=q_jq_{j+1}$ for all $j<L$. This is two-to-one mapping because for any $\vec{s}$ one has two $\vec{q}$'s such that $\vec{q}_+=(1,s_1,s_1s_2,\ldots,s_1s_2\ldots s_{L-1})$ and $\vec{q}_-=-\vec{q}_+$ differ by global inversion. This sets additional equivalence condition for subspace labels $(\vec{r},\vec{s})$: two subspaces $(\vec{r},\vec{u})$ and $(\vec{r},\vec{v})$ are equivalent if two strings $(1,u_1,u_1u_2,\ldots,u_1u_2,\ldots,u_{L-1})$ and $(1,v_1,v_1v_2,\ldots,v_1v_2,\ldots,v_{L-1})$ are related by translations or by a global inversion. For convenience let us call these two vectors TI (translation-inversion) related. Lattice translations along the columns set the same equivalence condition for $\vec{r}$ labels. Thus full equivalence conditions for subspace labels of the QCM are: (1) for $\alpha=\frac{1}{2}$ two subspaces $(\vec{r},\vec{s})$ and $(\vec{u},\vec{v})$ are equivalent if $\vec{r}$ is TI related with $\vec{u}$ and $\vec{s}$ with $\vec{v}$ or if $\vec{r}$ is TI related with $\vec{v}$ and $\vec{s}$ with $\vec{u}$. (2) For $\alpha\neq\frac{1}{2}$ two subspaces $(\vec{r},\vec{s})$ and $(\vec{u},\vec{v})$ are equivalent if $\vec{r}$ is TI related with $\vec{u}$ and $\vec{s}$ with $\vec{v}$. We have verified that no other equivalence conditions exist between the subspaces by numerical Lanczos diagonalizations for lattices of sizes up to 6×6 so we can change all *if* statements above into *if and only if* ones.

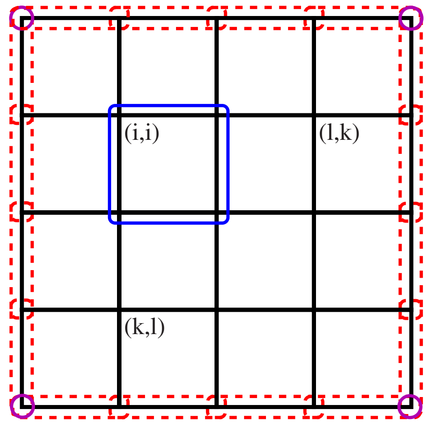

FIG. 2. (Color online) Schematic view of the z part of the reduced ground subspace Hamiltonian (8): circles in the corners stand for $\tilde{Z}_{i,j}$ spin operators related to the site (i,j), dashed (red) frames are $\tilde{Z}\tilde{Z}$ operator products acting on the boundaries of the lattice, and solid (blue) square stands for one of the plaquette $\tilde{Z}\tilde{Z}\tilde{Z}\tilde{Z}$ spin operators. The exemplary three sites in the identity (10) are: (i,i), (k,l), and (l,k).

IV. HIDDEN DIMER ORDER

Due to the symmetries of the QCM Eq. (1) only $\langle Z_{i,j}Z_{i,j+d}\rangle$ and $\langle X_{i,j}X_{i+d,j}\rangle$ spin correlations are finite $(d>0)$. This suggests that the entire spin order concerns *pairs of spins* from one row (column) which could be characterized by four-point correlation functions of the dimer-dimer type. Indeed, examining such quantities for finite QCM clusters via Lanczos diagonalization we observed certain surprising symmetry: for any α dimer-dimer correlators $\langle \mathcal{D}_{i,j}\mathcal{D}_{k,l}\rangle$ with $\mathcal{D}_{i,j} \equiv X_{i,j}X_{i+1,j}$, are invariant under the reflection of the second dimer with respect to the diagonal passing through site (i,j), see left panel of Fig. 1. This general relation between correlation functions of the QCM will be proved below.

We will prove that in the ground state of the QCM for any two sites (i,j) and (k,l) and for any $0<\alpha<1$

$$\langle X_{i,j}X_{i+1,j}X_{k,l}X_{k+1,l}\rangle \equiv \langle X_{i,j}X_{i+1,j}X_{l-\delta,k+\delta}X_{l-\delta+1,k+\delta}\rangle, \quad (5)$$

where $\delta=j-i$,[15] i.e., the second dimer is reflected with respect to the diagonal. To prove Eq. (5) let us transform again the effective Hamiltonian (4) in the ground subspace $(r_i \equiv s_i \equiv 1)$ introducing new spin operators

$$Z'_{i,j}=\tilde{Z}_{i,j}\tilde{Z}_{i,j+1}, \quad X'_{i,j}=\prod_{r=1}^{j}\tilde{X}_{i,r} \quad (6)$$

with $i,j=1,\ldots,L-1$ and $\tilde{Z}_{i,L}\equiv 1$. This yields to

$$\tilde{H}_x=\sum_{i=1}^{L-1}\sum_{j=1}^{L-1}\tilde{X}_{i,j}+\prod_{i=1}^{L-1}\prod_{j=1}^{L-1}\tilde{X}_{i,j}+\sum_{i=1}^{L-1}\prod_{j=1}^{L-1}\tilde{X}_{i,j}+\sum_{i=1}^{L-1}\prod_{j=1}^{L-1}\tilde{X}_{j,i}, \quad (7)$$

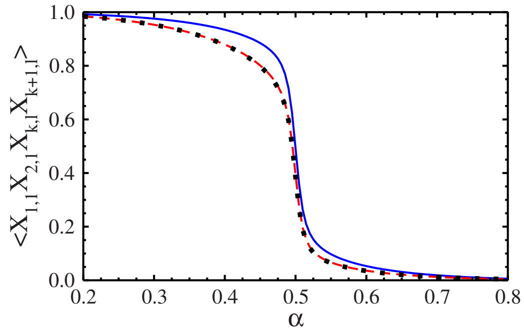

FIG. 3. (Color online) Two-dimer $\langle X_{1,1}X_{2,1}X_{k,l}X_{k+1,l}\rangle$ correlations for $L=6$ and $0.2<\alpha<0.8$: $(k,l)=(1,2)$, (1,3), and (1,4) are shown by solid, dashed, and dotted line.

$$\tilde{H}_z = \sum_a \left\{ \sum_b \tilde{Z}_{a,b} + \sum_{i=1}^{L-2} (\tilde{Z}_{a,i}\tilde{Z}_{a,i+1} + \tilde{Z}_{i,a}\tilde{Z}_{i+1,a}) \right\} + \sum_{i=1}^{L-2}\sum_{j=1}^{L-2} \tilde{Z}_{i,j}\tilde{Z}_{i,j+1}\tilde{Z}_{i+1,j}\tilde{Z}_{i+1,j+1}, \quad (8)$$

where $a,b=1,L-1$. Due to the spin transformations Eqs. (2), (3), and (6), $\tilde{X}_{i,j}$ operators are related to the original bond operators by $X_{i,j}X_{i+1,j}=\tilde{X}_{i,j}$, which implies that

$$\langle X_{i,j}X_{i+1,j}X_{k,l}X_{k+1,l}\rangle = \langle \tilde{X}_{i,j}\tilde{X}_{k,l}\rangle. \quad (9)$$

Because of the PBC, all original $X_{i,j}$ spins are equivalent, so we choose $i=j$. The x part, Eq. (7), of the Hamiltonian is completely isotropic. Note that the z part, Eq. (8), would also be isotropic without the boundary terms (see Fig. 2); the effective Hamiltonian in the ground subspace has the symmetry of a square. Knowing that in the ground state we have only Z_2 degeneracy, one finds

$$\langle \tilde{X}_{i,i}\tilde{X}_{k,l}\rangle \equiv \langle \tilde{X}_{i,i}\tilde{X}_{l,k}\rangle \quad (10)$$

for any i and (k,l). This proves the identity (5) for $\delta=0$; $\delta \neq 0$ case follows from lattice translations along rows.

The nontrivial consequences of Eq. (10) are: (i) *hidden dimer order* in the ground state of the QCM, i.e., an "isotropic" behavior of the two-pair correlator in spite of anisotropic interactions in the entire range of $0<\alpha<1$ (see Fig. 3) and (ii) long-range two-site $\langle X_{i,j}X_{i+d+1,j}\rangle$ correlations of range d along the columns which are equal to the multisite $\langle XX,\ldots,X\rangle$ correlations involving two neighboring rows, see right panel of Fig. 1. The latter follows from the symmetry properties of the transformed Hamiltonian Eqs. (7) and (8) applied to the multisite correlations

$$\langle \tilde{X}_{i,i}\tilde{X}_{i,i+1}\ldots\tilde{X}_{i,i+d}\rangle = \langle \tilde{X}_{i,i}\tilde{X}_{i+1,i}\ldots\tilde{X}_{i+d,i}\rangle. \quad (11)$$

V. MEAN-FIELD APPROXIMATION

The x part of the Hamiltonian obtained from Eq. (4) in case of open boundaries reads

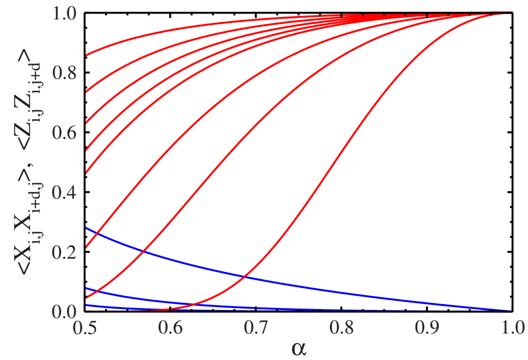

FIG. 4. (Color online) Long-range spin correlations of the 2D QCM, Eq. (1), obtained in the MF approach for $\alpha \geq \frac{1}{2}$. Lines starting from 1 at $\alpha=1$ are the $\langle Z_{i,j}Z_{i,j+d}\rangle$ correlations in Eq. (17) for $d=1,2,3,4,5,10,20,80$ while lines starting from 0 at $\alpha=1$ are the $\langle X_{i,j}X_{i+d,j}\rangle$ correlations in Eq. (16) with $d=1,2,3$; both in descending order.

$$H'_x = \sum_{i=1}^{L-1} \left\{ \sum_{j=1}^{L-2} X'_{i,j}X'_{i,j+1} + X'_{i,1} + r_i X'_{i,L-1} \right\} \quad (12)$$

and similarly for the z part. In the ground subspace ($r_i \equiv 1$) this resembles the original QCM, Eq. (1), but with linear boundary terms, which should not affect the ground-state properties in the thermodynamic limit and can be regarded as symmetry-breaking fields, resulting in finite values of $\langle X'_{i,j}\rangle$ and $\langle Z'_{i,j}\rangle$. Omitting the boundary terms in H'_x and H'_z and putting infinite L we recover the 2D QCM written in nonlocal primed spin operators. Now we can construct a MF splitting of the 2D lattice into (ferromagnetic) Ising chains in transverse field, taking common $\langle Z'\rangle \equiv \langle Z'_{i,j}\rangle$ as a Weiss field for each row i

$$\mathcal{H}'_i(\alpha) = -\sum_j \{(1-\alpha)X'_{i,j}X'_{i,j+1} + 2\alpha\langle Z'\rangle Z'_{i,j}\}. \quad (13)$$

In analogy to the compass ladder,[13] it can be solved by Jordan-Wigner transformation for each i

$$Z'_{i,j} = 1 - 2c^\dagger_{i,j}c_{i,j}, \quad (14)$$

$$X'_{i,j} = (c^\dagger_{i,j}e^{-i\pi/4} + c_{i,j}e^{i\pi/4})\prod_{r<j}(1-2c^\dagger_{i,r}c_{i,r}) \quad (15)$$

introducing fermion operators $\{c^\dagger_{i,j}\}$. The diagonalization of the free fermion Hamiltonian can be completed by performing first a Fourier transformation (from $\{j\}$ to $\{k\}$) and next a Bogoliubov transformation (for $k>0$): $\gamma^\dagger_k=\alpha^+_k c^\dagger_k+\beta^+_k c_{-k}$ and $\gamma^\dagger_{-k}=\alpha^-_k c^\dagger_k+\beta^-_k c_{-k}$, where $\{\alpha^\pm_k,\beta^\pm_k\}$ are eigenmodes of the Bogoliubov-de Gennes equation for the eigenvalues $\pm E_k$ (with $E_k>0$). The resulting ground state is a vacuum of $\gamma^\dagger_k$ fermion operators: $|\Phi_0\rangle=\Pi_{k>0}(\alpha^+_k+\beta^+_k c^\dagger_{-k}c^\dagger_k)|0\rangle$, which can serve to calculate correlations and the order parameter of the QCM in the MF approach. In agreement with numerical results (not shown), the only nonzero long-range two-site spin-correlation functions are: $\langle X_{i,j}X_{i+d,j}\rangle$ and $\langle Z_{i,j}Z_{i,j+d}\rangle$. For $d>1$ they can be represented as follows:

$$\langle X_{i,j}X_{i+d,j}\rangle = \langle X'_{i,j}X'_{i,j+1}\rangle^d, \quad (16)$$

$$\langle Z_{i,j}Z_{i,j+d}\rangle = \langle Z'_{i,j}Z'_{i,j+1}\ldots Z'_{i,j+d-1}\rangle^2. \tag{17}$$

Having solved the self-consistency equation for $\langle Z'\rangle = (1-2\langle n\rangle)$, with $\langle n\rangle = \frac{1}{L}\Sigma_{k>0}(\alpha_k^{-2}+\beta_k^{+2})$, one can easily obtain $\langle X'_{i,j}X'_{i,j+1}\rangle$, Eq. (16), for increasing α

$$\langle X'_{i,j}X'_{i,j+1}\rangle = \frac{2}{L}\sum_{k>0}\{\cos k(\alpha_k^{-2}+\beta_k^{+2}) + \sin k(\alpha_k^{-}\beta_k^{-} - \alpha_k^{+}\beta_k^{+})\}. \tag{18}$$

The nonlocal $\langle Z'_{i,j}Z'\ldots Z'_{i,j+d-1}\rangle$ correlations Eq. (17) are more difficult to find but they can be approximated by

$$\langle Z'_{i,j}Z'_{i,j+1}\ldots Z'_{i,j+d-1}\rangle = \prod_{k>0}\left\{\alpha_k^{+2}\left(1-2\frac{d}{L}\right)^2 + \beta_k^{+2}\right\}, \tag{19}$$

where $L\to\infty$ and $k=(2l-1)\frac{\pi}{L}$ with $l=1,2,\ldots,\frac{L}{2}$. This approximation is valid as long as $d \ll L$. One finds that the long-range $\langle Z_{i,j}Z_{i,j+d}\rangle$ correlations in Z-ordered phase at $\alpha \geq \frac{1}{2}$ show the absence of the Ising-type long-range order for $\alpha < 1$ (Fig. 4)—they decrease slowly with growing distance d or decreasing α.[16] In contrast, the $\langle X_{i,j}X_{i+d,j}\rangle$ correlations are significant only for nearest neighbors ($d=1$) and close to $\alpha = \frac{1}{2}$.

The advantage of this nonlocal MF approach for the QCM Eq. (1) over the standard one, which takes $\langle Z\rangle$ as a Weiss field, is that we do not break the $\{P_i, Q_j\}$ and Z_2 symmetries of the model. What more, thanks to numerical and analytical results we know that order parameter of the QCM is given by $\langle H_z\rangle$ (Ref. 4)—the quantity behaving more like $\langle Z'\rangle$ rather than $\langle Z\rangle$ (having $\langle Z\rangle > 0$ would mean long-range magnetic order). Another interesting feature of the Hamiltonian (1) is that it describes all nonlocal compass excitations over the ground state while the local ones manifest themselves by directions of symmetry-breaking fields. These nonlocal column (row) flips are especially interesting from the point of view of topological quantum computing[2] because they guarantee that the system is protected against local perturbations.

VI. CONCLUSIONS

On the example of the QCM, we argue that the properties of spin models which are not SU(2) symmetric can be uniquely determined by discrete symmetries such as parity. In this case conservation of spin parities in rows and columns, for x and z components of spins, makes the system in the ground-state behave according to a nonlocal Hamiltonian (4).[17] In the ground state most of the two-site spin correlations vanish and the two-dimer correlations exhibit the nontrivial hidden order. The excitations involve whole lines of spins in the lattice and occur in invariant subspaces which can be classified by lattice translations—the reduction in the Hilbert space achieved in this way is important for future numerical studies of the QCM and will play a role for spin models with similar symmetries. Finally, the nonlocal Hamiltonian containing symmetry-breaking terms suggests the MF splitting respecting conservation of parity and leading to the known physics of one-dimensional quantum Ising model describing correlation functions and the order parameter of the QCM.

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[15] The symmetry of Eq. (1) implies a similar relation for Z correlations with dimers along the horizontal bonds.

[16] At $\alpha = \frac{1}{2}$ the Z-ordered and X-ordered Ising-type phases of the QCM are degenerate, see e.g. Ref. 5.

[17] The nonlocal Hamiltonian is just the original QCM, Eq. (1), written in eigenbasis of $\{P_i, Q_j\}$ parities.