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 $(X_{i,i+1}X_{i+1,i},X_{i,i+1}X_{i+1,i})$ and $(X_{i,i+1}X_{i+1,i},X_{i,i+1}X_{i+1,i})$ in the ground state, which is independent of the actual interactions. This order coexists with Ising-like spin correlations which decay with distance.

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The quantum compass model (QCM) originates from the frustrated (Kugel-Khomskii) superexchange interaction in transition metal oxides with degenerate 3$d$ orbitals. Recent interest in this model is motivated by its interdisciplinarity 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. The QCM is dual to the models of frustrated superexchange and anisotropic interactions are varied through the isotropic point, as shown by an analytical method. The QCM is dual to the models of frustrated superexchange and anisotropic interactions are varied through the isotropic point.

In spite of several numerical studies 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. The 2D QCM shows a self-duality which might serve to reveal nontrivial hidden symmetries. In this Letter we employ exact spin transformations which allow us to discover a surprising hidden dimer order in the QCM which manifests itself by exact relations between four-point correlation functions in the ground state. We also demonstrate nonlocal mean-field splitting of the QCM in the ground subspace and determine spatial decay of spin correlations in the thermodynamic limit. Reduced Hamiltonian. — We consider the anisotropic ferromagnetic QCM for pseudospins $1/2$ on an $L \times L$ square lattice with periodic boundary conditions (PBC),

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

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 another operator. The QCM Eq. (1) can be written in common eigenbasis of $\{R_i, Q_j\}$ operators using:

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

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

where $\tilde{Z}_{i,j} \equiv 1$ and $X'_{i,j} \equiv 1$. One finds that the transformed Hamiltonian, $\mathcal{H}'(\alpha) = - (1-\alpha)H^x - \alpha H^z$, contains no $\tilde{X}_{i,j}$ and no $Z'_{i,j}$ operators so the corresponding $\tilde{Z}_{i,j}$ and $X'_{i,j}$ 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,

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

where $r = \prod_{i=1}^{L-1} r_i$, and new nonlocal $P'_1 = \prod_{j=1}^{L-1} X'_{p,j}$ operators originate from the PBC. The $z$-part $H'_z$ follows from $H'_x$ by lattice transposition $X'_{i,j} \rightarrow Z_{i,j}$ and by $r_i \rightarrow s_j = q_j q_{j+1}$. Ising variables $r_i$ and $s_j$ are the eigenvalues of the 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
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 (1) 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’s 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 \( j < \text{L} \) and \( Q_L \rightarrow Q_1 \). This implies that two subspaces \((\vec{r}, q_1, q_2, \ldots, q_L)\) and \((\vec{r}, q_1, q_2, \ldots, q_{L-1})\) are equivalent for all values of \( \vec{r} \) and \( q \). Now this result must be translated into the language of \((\vec{r}, \vec{s})\) labels, with \( s_j = q_j q_{j+1} \) for all \( j < \text{L} \). This is two-to-one mapping because for any \( s \)'s one has two \( q \)'s such that \( q_+ = (1, s_1, s_1 s_2, \ldots, s_1 s_2 \ldots s_{L-1}) \) and \( q_- = -q_+ \) 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 \((1, u_1, u_1 u_2, \ldots, u_1 u_2 \ldots u_{L-1})\) and \((1, v_1, v_1 v_2, \ldots, v_1 v_2 \ldots v_{L-1})\) 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 \( \vec{s} \) labels. Thus full equivalence conditions for subspace labels of the QCM are:

- 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 \( \vec{u} \).
- 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 \( 6 \times 6 \), so we can change all \( if \) statements above into \( i f \ and \ only \ if \) ones.

Hidden dimer order. — Due to the symmetries of the QCM Eq. (1) only \( \langle Z_{i,j} Z_{i,j+1} \rangle \) 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 \( \alpha \) dimer-dimer correlators \(\{D_{i,j} \langle \tilde{D}_{k,l} \rangle \}\), with \( D_{i,j} = X_{i,j} X_{i+1,j} \), 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 \( 0 < \alpha < 1 \):

\[
\langle X_{i,j} X_{i+1,j} X_{k,l} X_{k+1,l} \rangle = \langle X_{i,j} X_{i+1,j} X_{l-\delta, k+\delta} X_{l-\delta+1, k+\delta} \rangle,
\]

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

\[
Z_{i,j} = \tilde{Z}_{i,j} Z_{i,j+1}, \quad X_{i,j} = \prod_{r=1}^j \tilde{X}_{i,r},
\]

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

\[
\tilde{H}_x = L-1 \sum_{i=1}^{L-1} \sum_{j=1}^{L-1} \tilde{X}_{i,j} + \sum_{i=1}^{L-1} \sum_{j=1}^{L-1} \tilde{X}_{i,j} + \tilde{X}_{j,i} + \tilde{X}_{j,i} + \tilde{X}_{j,i} + \tilde{X}_{j,i},
\]

\[
\tilde{H}_z = L-2 \sum_{i=1}^{L-2} \sum_{j=1}^{L-2} \tilde{Z}_{i,j} + \sum_{i=1}^{L-2} \sum_{j=1}^{L-2} \tilde{Z}_{i,j} + \tilde{Z}_{i,j} + \tilde{Z}_{i,j} + \tilde{Z}_{i,j} + \tilde{Z}_{i,j},
\]

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

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

Because of the PBC, all original $X_{i,j}$ spins are equivalent, so we choose $i = j$. The $x$-part $[7]$ of the Hamiltonian is completely isotropic. Note that the $z$-part $[3]$ 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

$$\langle \hat{X}_{i,i} \hat{X}_{k,l} \rangle = \langle \hat{X}_{i,i} \hat{X}_{k,l} \rangle,$$  \hspace{1cm} (10)

for any $i$ and $(k, l)$. This proves the identity $[3]$ 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 correlations of range $d$ along the columns which are equal to the multi-site $\langle XX \ldots X \rangle$ correlations involving two neighboring rows, see right panel of Fig. 1. The latter follows from the symmetry properties of the transformed Hamiltonian $[7,3]$ applied to the multi-site correlations:

$$\langle \hat{X}_{i,i} \hat{X}_{i+1,i} \ldots \hat{X}_{i+d,i} \rangle = \langle \hat{X}_{i,i} \hat{X}_{i+1,i} \ldots \hat{X}_{i+d,i} \rangle.$$  \hspace{1cm} (11)

**Mean-field approximation.** — The $x$-part of the Hamiltonian obtained from Eq. (11) in case of open boundaries reads:

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

and similarly for the $z$-part. In the ground subspace ($\epsilon_1 = 1$) 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 $\langle Z' \rangle \equiv \langle Z'_{i,j} \rangle$ as a Weiss field for each row $i$:

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

In analogy to the compass ladder $[23]$ it can be solved by Jordan-Wigner transformation for each $i$:

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

$$X'_{i,j} = \left( c^+_{i,j} e^{-i\pi \gamma_j} + c_{i,j} e^{i\pi \gamma_j} \right) \prod_{r<j} (1 - 2c^+_{i,r} c_{i,r}),$$  \hspace{1cm} (15)

introducing fermion operators $\{c^+_{i,j}\}$. 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 $k > 0$):

$$\gamma_k = \alpha_k e_k + \beta_k c_{-k} \text{ and } \gamma_{-k} = \alpha_k - e_k + \beta_k c_{-k},$$

where $\{\alpha_k, \beta_k\}$ 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 $\gamma_k$ fermion operators: $\langle \Phi_0 \rangle = \prod_{k>0} (\alpha_k^+ + \beta_k^+ c_{-k}^+ c_k)|0\rangle$, 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:

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

$$\langle Z_{i,j} Z_{i,j+d} \rangle = \langle Z'_{i,j} Z'_{i,j+1} \ldots Z'_{i,j+d-1} \rangle^2.$$  \hspace{1cm} (17)
Having solved the self-consistency equation for $\langle Z' \rangle = (1 - 2\langle n \rangle)$, with $\langle n \rangle = 1/2$ \( \sum_{k>0} \left( \alpha_k^{-2} + \beta_k^2 \right) \), one can easily obtain $\langle X'_{i,j} X'_{i,j+1} \rangle$ \cite{19} for increasing $\alpha$:

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

The nonlocal $\langle Z'_i Z'_i \cdots Z'_{i,j+d-1} \rangle$ correlations are more difficult to find but can be approximated by

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

where $L \to \infty$ and $k = (2l-1)\pi$ with $l = 1, 2, \ldots, \frac{1}{2}$. This approximation is valid as long as $d \ll L$. One finds that the long range $\langle Z'_i Z'_i \rangle$ correlations in $Z$-ordered phase at $\alpha > 1/2$ show the absence of the Ising-like long range order for $\alpha < 1$ (Fig. 3) — they decrease slowly with growing distance $d$ or decreasing $\alpha$ \cite{19}. In contrast, the $\langle X_{i,j} X_{i+d,j} \rangle$ correlations are significant only for nearest neighbors $(d = 1)$ and close to $\alpha = 1/2$.

The advantage of this nonlocal MF approach for the QCM Eq. (1) over the standard one, which takes $\langle X \rangle$ 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 $\langle H_0 \rangle$ — the quantity behaving more like $\langle Z' \rangle$ rather than $\langle X \rangle$ (having $\langle Z \rangle > 0$ would mean long range magnetic order!). Another interesting feature of the Hamiltonian \cite{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\cite{20} because they guarantee that the system is protected against local perturbations.

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 like 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 \cite{1} \cite{2}. 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 of 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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The symmetry of Eq. (1) implies a similar relation for $Z$-correlations with dimers along the horizontal bonds.

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

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