Systematic Derivation of Order Parameters through Reduced Density Matrices

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A systematic method for determining order parameters for quantum many-body systems on lattices is developed by utilizing reduced density matrices. This method allows one to extract the order parameter directly from the wave functions of the degenerate ground states without the aid of empirical knowledge, and thus opens a way to explore unknown exotic orders. The applicability of this method is demonstrated numerically or rigorously in models that are considered to exhibit dimer, scalar chiral, and topological orders.

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Determining order parameters is one of the most important issues in the study of many-body systems. A suitably chosen order parameter for a symmetry-breaking phase provides an intuitive picture of the long range order and is the necessary starting point of the Landau-Ginzburg-type effective description of the system [1]. Combined with Wilson's idea of renormalization group [2], such an effective theory becomes a powerful tool in analyzing the nature of the phase transitions to other phases.

In spite of the importance of this issue, a general method to obtain an order parameter in a given model is not available. The knowledge of previous examples suggests some candidates, but this empirical method may fail in the case of a new order. Especially in a system with strong frustration and/or quantum fluctuation, the order parameter can be quite nontrivial. With more examples of exotic orders becoming a subject of great theoretical and experimental interest, a *systematic* method for determining an order parameter would be strongly desired.

In this Letter, we present a solution to the quantum version of this problem. In the quantum case, when a symmetry of the Hamiltonian is broken spontaneously in the thermodynamic limit, there appear degenerate ground states (GS). An order parameter can be identified with an operator that distinguishes the degenerate GSs. The central idea of our method is to search such an operator by comparing the reduced density matrices (RDM) of the degenerate GSs for various subareas of the system. A RDM efficiently encapsulates the expectation values of all the operators on the concerned area. If the RDMs of the GSs are different on an area, an order parameter can be defined on that area. In this way, we can determine the smallest area on which an order parameter can be defined. Moreover, for the resultant area, we can construct an ''optimal'' order parameter from the RDMs. This method can be applied to the low-energy eigenstates obtained by exact diagonalization, for instance, and can reveal the order parameter without bias.

We demonstrate the effectiveness of this approach in concrete models. We consider the multiple-spin exchange model on the ladder and detect dimer and scalar chiral orders that have been found in previous studies [3,4]. We also consider a resonating valence bond (RVB) liquid in a solvable quantum dimer model (QDM) [5] and rigorously show that its GSs cannot be characterized by *any* local order parameter [6]. Namely, the model unambiguously is shown to possess a topological order.

Methodology.—Suppose that we have obtained the low-energy spectrum and eigenstates of finite-size systems by exact diagonalization, for instance. In a phase breaking a *discrete* symmetry, we find a finite number of nearly degenerate GSs that become asymptotically degenerate when increasing the system size. Each of these states does not break any symmetry of the Hamiltonian, but its quantum numbers indicate what symmetries are broken in the thermodynamic limit.

Let us focus on the simplest case: the Hamiltonian is invariant under the translation by one lattice spacing, $\mathcal{T}$, is real in terms of $\{S_j^z\}$ basis, and exhibits doubly degenerate GSs, $|\Phi_1\rangle$ and $|\Phi_2\rangle$, with momenta $k = 0$ and π, respectively. In this case, we expect the breaking of the translational symmetry (doubling of the unit cell) in the thermodynamic limit. We set $|\Phi_1\rangle$ and $|\Phi_2\rangle$ real, i.e., $\mathcal{K}|\Phi_i\rangle = |\Phi_i\rangle$ $(i = 1, 2)$, where $\mathcal{K}$ denotes the time-reversal operator that converts every component of a vector into its complex conjugate in terms of the $\{S_j^z\}$ basis [7].

We construct the symmetry-breaking GSs, $|\Psi_1\rangle$ and $|\Psi_2\rangle$, as linear combinations of $|\Phi_1\rangle$ and $|\Phi_2\rangle$. We require that they be orthogonal ($\langle\Psi_1|\Psi_2\rangle = 0$) and be exchanged under $\mathcal{T}$ ($\mathcal{T}|\Psi_{1(2)}\rangle \propto |\Psi_{2(1)}\rangle$). There are still two possibilities, depending on whether the time-reversal symmetry is broken ($\mathcal{K}|\Psi_{1(2)}\rangle \propto |\Psi_{2(1)}\rangle$) or not ($\mathcal{K}|\Psi_{1(2)}\rangle \propto |\Psi_{1(2)}\rangle$). For each case, the symmetry-breaking GSs are constructed as

$$\begin{aligned} &|\Psi_{1,2}\rangle = (|\Phi_1\rangle \pm |\Phi_2\rangle)/\sqrt{2} \ (\mathcal{K} - \text{unbreaking case}), \\ &|\Psi_{1,2}\rangle = (|\Phi_1\rangle \pm i|\Phi_2\rangle)/\sqrt{2} \ (\mathcal{K} - \text{breaking case}). \end{aligned} \tag{1}$$

Here both possibilities have to be examined since, due to

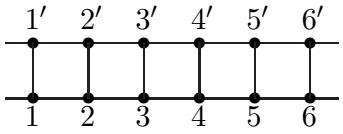

FIG. 1. Numbering of the sites on the two-leg ladder.

the antiunitarity of the time-reversal operator, we do not know from the quantum numbers whether the system breaks the time-reversal symmetry or not.

Next we search an operator that distinguishes the symmetry-breaking GSs by comparing the RDMs $\rho_\Omega^i = \mathrm{Tr}_{\bar{\Omega}}|\Psi_i\rangle\langle\Psi_i|$ $(i = 1, 2)$, where Ω is an area in the system and $\bar{\Omega}$ its complement. To quantify to what extent the two RDMs are different, we introduce a measure as

$$\mathrm{diff}\,(\rho_\Omega^1, \rho_\Omega^2) \equiv \max_{|\mathcal{O}_\Omega|\le 1} |\mathrm{Tr}_\Omega(\mathcal{O}_\Omega \rho_\Omega^1) - \mathrm{Tr}_\Omega(\mathcal{O}_\Omega \rho_\Omega^2)|, \tag{2}$$

where $\mathcal{O}_\Omega$ is a variational (Hermitian) operator on Ω satisfying $|\langle\psi|\mathcal{O}_\Omega|\psi\rangle| \le 1$ for any normalized vector $|\psi\rangle$. If $\mathrm{diff}(\rho_\Omega^1, \rho_\Omega^2) > 0$, there exists an operator on Ω distinguishing $|\Psi_1\rangle$ and $|\Psi_2\rangle$. This measure has the following useful properties: (a) normalization to a definite range $0 \le \mathrm{diff}(\rho_\Omega^1, \rho_\Omega^2) \le 2$, for an arbitrary area Ω; (b) monotonicity: if an area Λ completely contains an area Ω, we have $\mathrm{diff}(\rho_\Omega^1, \rho_\Omega^2) \le \mathrm{diff}(\rho_\Lambda^1, \rho_\Lambda^2)$.

Using the eigenvalues $\{\lambda_j\}$ and the eigenvectors $\{|j\rangle\}$ of $\Delta\rho_\Omega \equiv \rho_\Omega^1 - \rho_\Omega^2$, Eq. (2) can be simplified as

$$\mathrm{diff}\,(\rho_\Omega^1, \rho_\Omega^2) = \max_{|\mathcal{O}_\Omega|\le 1} \left| \sum_j \lambda_j \langle j|\mathcal{O}_\Omega|j\rangle \right| = \sum_j |\lambda_j|. \tag{3}$$

Here the maximization is done by the optimal order parameter:

$$\mathcal{O}_\Omega^{(\mathrm{opt})} = \sum_j |j\rangle \mathrm{sgn}\lambda_j \langle j|, \tag{4}$$

where $\mathrm{sgn}\lambda_j$ is the sign of λ_j if $\lambda_j \neq 0$ and is zero if $\lambda_j = 0$. Both the measure and the optimal order parameter can be calculated by (numerically) diagonalizing $\Delta\rho_\Omega$. As we have discussed above, generally we have to examine both the $\mathcal{K}$-unbreaking and $\mathcal{K}$-breaking combinations in Eq. (1). In the following, we denote the measure (2) for the $\mathcal{K}$-unbreaking and $\mathcal{K}$-breaking cases as "diff1" and "diff2," respectively.

The generalization of this method to systems with more than two degenerate GSs can be formulated as an optimization problem, which will be presented elsewhere.

Simple examples.—To illustrate this method, let us consider two simple examples, Néel and dimer orders. The corresponding symmetry-unbreaking GSs are, respectively, given by

$$|\Psi_{1,2}^{\mathrm{N\acute{e}el}}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\cdots\rangle \pm |\downarrow\uparrow\cdots\rangle), \tag{5}$$

$$|\Psi_{1,2}^{\mathrm{dimer}}\rangle = \frac{1}{\sqrt{2}}(|s_{12}\rangle\cdots|s_{N-1,N}\rangle \pm |s_{23}\rangle\cdots|s_{N,1}\rangle), \tag{6}$$

where $|s_{ij}\rangle$ denotes a singlet bond. For the Néel order, $\mathrm{diff}1 = 2$ for a 1-site area $\{1\}$ while diff2 is zero for the same area. Thus, the optimal order parameter should be constructed from the RDMs of the $\mathcal{K}$-unbreaking GSs on $\{1\}$, resulting in $\mathcal{O}_{\{1\}}^{(\mathrm{opt})} = 2S_1^z$. For the dimer order, on the other hand, both diff1 and diff2 are zero for $\{1\}$, but we find $\mathrm{diff}1 = 3/2 > 0$ for a 2-site area $\{1, 2\}$. The resultant optimal order parameter (4) for this area is $\mathcal{O}_{\{1,2\}}^{(\mathrm{opt})} = 2\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 + 1/2$. We have obtained the expected order parameters for both of the simple examples.

Actually, in order to establish the presence (or absence) of an order parameter on a given finite area, the measure "diff" (2) has to be defined in the thermodynamic limit. However, in most of the applications, especially in numerical calculations, we are able to calculate only the corresponding quantity in finite systems. We expect that, in a gapped system, the diff should converge exponentially to the true value, when the system size is taken to infinity. While the systematic study of such a finite-size effect is outside the scope of this Letter, the following application demonstrates the usefulness of our measure even in numerical diagonalization of relatively small systems.

Application I.—We consider the 2-spin and 4-spin exchange model with spin $S = 1/2$ on the two-leg ladder:

$$\mathcal{H} = \cos\theta \sum_{-} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \sin\theta \sum_{\square} (P_4 + P_4^{-1}), \tag{7}$$

where the two summations run over the (vertical and horizontal) bonds and the squares, respectively. According to recent analyses [3,4], two ordered phases breaking the translational symmetry have been found: the staggered dimer phase ($0.07\pi \lesssim \theta < \theta_c$) and the scalar chiral phase ($\theta_c < \theta \lesssim 0.39\pi$), separated by the exact self-dual point $\theta_c = \tan^{-1}(1/2) \simeq 0.1476\pi$ [4]; see Fig. 2(a) below.

In both regions, the finite-size spectra obtained from exact diagonalization exhibit two nearly degenerate singlet GSs with quantum numbers, $(k_x, k_y, \sigma) = (0, 0, 1)$ and $(\pi, \pi, -1)$, where (k_x, k_y) denotes the momentum and σ the reflection with respect to a rung. We constructed symmetry-breaking GSs from these states and calculated diff for various areas; see Table I. At $\theta = 0.12\pi$, the minimum area required to find an order parameter is $\{1, 2\}$, and the time-reversal symmetry is unbroken. Since $\Delta\rho_{\{1,2\}}$ is symmetric under the spin rotations and the time reversal, it must be proportional to $\boldsymbol{S}_1 \cdot \boldsymbol{S}_2$, and hence the optimal order parameter is $\mathcal{O}_{\{1,2\}}^{(\mathrm{opt})} = 2\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 + 1/2$. At $\theta = 0.19\pi$, the minimum area consists of three sites (e.g., $\{1, 2, 1'\}$) and the time-reversal symmetry is broken. Since $\Delta\rho_{\{1,2,1'\}}$ is symmetric under the spin rotations and antisymmetric under the time reversal, we have $\Delta\rho_{\{1,2,1'\}} \propto \boldsymbol{S}_1 \cdot (\boldsymbol{S}_2 \times \boldsymbol{S}_{1'})$, and hence $\mathcal{O}_{\{1,2,1'\}}^{(\mathrm{opt})} = \frac{4}{\sqrt{3}} \boldsymbol{S}_1 \cdot (\boldsymbol{S}_2 \times \boldsymbol{S}_{1'})$. In

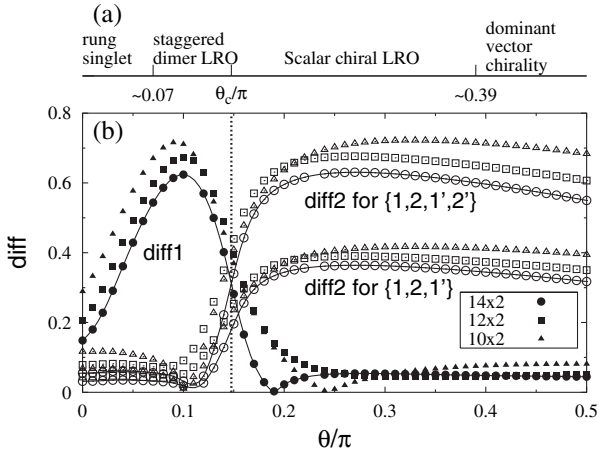

FIG. 2. (a) Phase diagram obtained from earlier studies [3,4]. (b) Values of diff1 and diff2 for the fixed areas, $\{1, 2, 1'\}$ and $\{1, 2, 1', 2'\}$, versus θ. The values of diff1 (filled symbols) for the two areas are exactly the same. As for diff2 (open symbols), the upper and the lower points refer to $\{1, 2, 1', 2'\}$ and $\{1, 2, 1'\}$, respectively. Lines are guides to eyes. The vertical dotted straight line represents the self-dual point θ_c. Our calculation assumes a quasidegeneracy of the GSs and is therefore invalid for $\theta \lesssim 0.07\pi$ and $0.39\pi \lesssim \theta$.

this way, we have *derived* the dimer and the scalar chiral operators as the appropriate order parameters in a systematic way.

In Fig. 2(b), θ dependence of diff1 and diff2 are shown for fixed areas. Rapid changes in the values of diff can be seen around the self-dual point θ_c, confirming the phase transition between the two ordered phases. For $\{1, 2, 1', 2'\}$, the values of diff1 and diff2 cross exactly at θ_c. For $\{1, 2, 1'\}$, the crossing of diff1 and diff2 deviates from θ_c but approaches it when increasing the system size. In general, such a crossing indicates a phase transition between ordered phases that cannot be distinguished by the GS quantum numbers.

Application II.—We next consider a solvable QDM on the kagome lattice introduced recently [5] (for a review, see also section 5 of Ref. [8]), which is one of the microscopic models realizing a short-ranged (so-called $\mathbb{Z}_2$) RVB liquid. This model also provides an example of a solvable Hamiltonian [9] for a topological quantum bit based on a QDM [10]. Before applying our method, we briefly review the definition of this model and some basic concepts.

This model is simply expressed in terms of the arrow representation [11] of dimer coverings defined in the following way. The sites of the kagome lattice K can be identified with the centers of the bonds of the hexagonal lattice H. For a dimer covering of K, we assign orientations (arrows) to the bonds of H so that the arrow on each site of K points towards the interior of the triangle of K where the dimer occupying the site is [see Fig. 3(a)]. As a consequence, the number of incoming arrows is even (0 or 2) at every triangle. Let S be the set of arrow configurations satisfying this local parity constraint at every triangle. There is a one-to-one correspondence between S and the set of all dimer coverings.

We define $\tau^z(i)$ as the operator that flips the arrow on the site i of K. Dimer movements can be represented as loop products of τ^z operators. The Hamiltonian we consider is the sum of the loop operators around the hexagons h of K: $\mathcal{H} = -\sum_h \prod_{\alpha=1}^{6} \tau^z(i_{h,\alpha})$, where $i_{h,\alpha}$ are the six sites of the hexagon h.

If this model is defined on a surface with a *nontrivial topology* (cylinder, torus, etc.), arrow configurations in S can be grouped into topological sectors that are not mixed by any succession of local dimer moves. From now on, we concentrate on the case of the cylinder for simplicity (but all the results can be easily generalized to other topologies). We draw a cut Δ (passing through the bonds of H) going from the top to the bottom of the cylinder. We classify arrow configurations into two topological sectors, S^+ and S^-, depending on whether the number of arrows crossing Δ to the right is even or odd. The spectrum can be determined separately in each sector. Using the standard Rokhsar-Kivelson argument [12], one can show that the ground state in a given sector is exactly the equal-amplitude superposition of all dimer coverings (arrow configurations) belonging to that sector:

TABLE I. Values of diff for various areas in the 14×2 ladder. The points, $\theta = 0.12\pi$ and 0.19π, are the representative points, respectively, in the staggered dimer and the scalar chiral phases found previously [3,4]. The sites are numbered as shown in Fig. 1. Some zeros (indicated by $*$) are exact consequences of the symmetries.

	$\theta = 0.12\pi$		$\theta = 0.19\pi$	
Area Ω	diff1	diff2	diff1	diff2
$\{1\}$	0^*	0^*	0^*	0^*
$\{1, 2\}$	0.5698	0^*	0.0029	0^*
$\{1, 1'\}$	0^*	0^*	0^*	0^*
$\{1, 2'\}$	0^*	0^*	0^*	0^*
$\{1, 2, 1'\}$	0.5698	0.0267	0.0029	0.3340
$\{1, 2, 3\}$	0.6579	0.0670	0.0033	0.2365
$\{1, 2, 1', 2'\}$	0.5698	0.0462	0.0029	0.5785

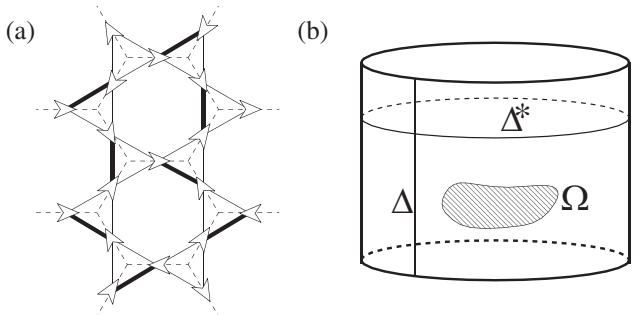

FIG. 3. (a) Dimer covering and arrow representation. (b) Local area Ω on the cylinder. The cut Δ and the loop Δ^* can be drawn so as not to touch Ω.

$$|\mu\rangle = \frac{1}{\sqrt{|S^\mu|}} \sum_{a \in S^\mu} |a\rangle, \qquad \mu = +, -. \tag{8}$$

These two states are exactly degenerate and form a two-dimensional GS subspace.

Now we consider the RDM of a state $|\Psi\rangle$ in the GS subspace and discuss how it depends on the choice of $|\Psi\rangle$. The area Ω is given as a set of bonds of H. The RDM $\rho_\Omega = \mathrm{Tr}_{\bar{\Omega}} |\Psi\rangle\langle\Psi|$ is defined by tracing out the degrees of freedom (arrows) on $\bar{\Omega}$:

$$\langle a_1|\rho_\Omega|a_2\rangle = \sum_{\bar{a}} \langle a_1, \bar{a}|\Psi\rangle\langle\Psi|a_2, \bar{a}\rangle, \tag{9}$$

where a_1 and a_2 are arrow configurations on Ω and the sum is over all the arrow configurations $\bar{a}$ on $\bar{\Omega}$. By expressing $|\Psi\rangle = \sum_\mu \alpha_\mu |\mu\rangle$ with $\sum_\mu |\alpha_\mu|^2 = 1$, ρ_Ω can be expanded as

$$\rho_\Omega = \sum_{\mu,\nu} \alpha_\mu \alpha_\nu^* \mathcal{M}_\Omega^{\mu\nu}, \qquad \mathcal{M}_\Omega^{\mu\nu} = \mathrm{Tr}_{\bar{\Omega}} |\mu\rangle\langle\nu|. \tag{10}$$

First, we assume that Ω is a (finite) local area; see Fig. 3(b). We prove the following relations:

$$\mathcal{M}_\Omega^{+-} = 0, \qquad \mathcal{M}_\Omega^{\mu\nu} = \mathcal{M}_\Omega^{\bar{\mu}\,\bar{\nu}}, \tag{11}$$

where the overbars represent the sign flip. To prove the first relation, we choose the cut Δ so as not to touch Ω. Then the parity along Δ for an arrow configuration depends only on its part on $\bar{\Omega}$. Let us consider the matrix element of $\mathcal{M}_\Omega^{+-}$: $\langle a_1|\mathcal{M}_\Omega^{+-}|a_2\rangle = \sum_{\bar{a}} \langle a_1, \bar{a}|+\rangle\langle -|a_2, \bar{a}\rangle$. Since the two configurations, $(a_1, \bar{a})$ and $(a_2, \bar{a})$, have common parity, $\langle a_1, \bar{a}|+\rangle$ and $\langle -|a_2, \bar{a}\rangle$ cannot be nonzero at the same time, and hence we obtain $\mathcal{M}_\Omega^{+-} = 0$.

To prove the second relation in Eq. (11), we draw a loop Δ^* (passing along the bonds of H) encircling the cylinder so as not to touch the area Ω. We introduce a loop operator along Δ^*: $T^z_{\Delta^*} = \Pi_{i \in \Delta^*} \tau^z(i)$. This operator acts only on $\bar{\Omega}$ and maps $|\pm\rangle$ to $|\mp\rangle$, showing $\mathcal{M}_\Omega^{\mu\nu} = \mathrm{Tr}_{\bar{\Omega}}(T^z_{\Delta^*}|\bar{\mu}\rangle \times \langle\bar{\nu}|T^z_{\Delta^*}) = \mathrm{Tr}_{\bar{\Omega}}(|\bar{\mu}\rangle\langle\bar{\nu}|(T^z_{\Delta^*})^2) = \mathcal{M}_\Omega^{\bar{\mu}\,\bar{\nu}}$.

From Eqs. (10) and (11), we see that ρ_Ω is independent of the choice of $|\Psi\rangle$. Thus, no order parameter can be defined on an arbitrary local area. In the context of topological quantum bit based on QDMs [9,10], this shows the stability of quantum information against external noises (coupling locally to dimers).

The situation is different if Ω has a nontrivial topology, namely, extends from the top to the bottom of the cylinder (case A) or encircles the cylinder (case B). In case A, we can choose the cut Δ inside Ω. Then the parity along Δ can be expressed as the operator acting on Ω and distinguishes the different topological sectors. It can be considered as a nonlocal order parameter distinguishing $|+\rangle$ and $|-\rangle$. Similarly, in case B, two states $(|+\rangle \pm |-\rangle)/\sqrt{2}$ are distinguished by the loop operator $T^z_{\Delta^*}$ with Δ^* defined inside Ω.

We have shown that the GSs of this QDM cannot be distinguished by any local operator but by nonlocal operators defined on areas with nontrivial topologies. We comment that a similar result has been shown without using RDMs by Ioffe and Feigel'man [13] in their study on a related model. We stress, however, that our formulation based on RDMs has an advantage in its generality. As demonstrated in the ladder model, it can be applied to models without exact solutions, by combining it with numerical calculation, for example.

Conclusions.—We have developed a method that can determine order parameters without using any empirical knowledge. The two applications confirmed its applicability to exotic orders and, especially, its relevance for analyzing topological orders. We expect that our method will shed some light on the controversies in some frustrated quantum antiferromagnets (see Ref. [8] and references therein), e.g., the $J_1 - J_2$ model on the square lattice and the multiple-spin exchange model on the triangular lattice.

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