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 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 which 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. Combined with Wilson’s idea of renormalization group, 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 non-trivial. 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 which 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 will demonstrate the effectiveness of this approach in concrete models. We will consider the multiple-spin exchange model on the ladder and detect dimer and scalar chiral orders which have been found in previous studies. We will also consider a resonating valence bond (RVB) liquid in a solvable quantum dimer model and rigorously show that its GSs cannot be characterized by any local order parameter. Namely, the model will unambiguously be 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 which 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 \( \{ S^z \} \)-basis, and exhibits doubly-degenerate GSs, \( | \Phi_1 \rangle \) and \( | \Phi_2 \rangle \), with momenta \( k = 0 \) and \( \pi \), 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 which converts every component of a vector into its complex conjugate in terms of \( \{ S^z \} \)-basis.

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 \( \mathcal{T} \) \( \langle \mathcal{T}| \Psi_{1(2)} \rangle \propto | \Psi_{2(1)} \rangle \). There are still two possibilities, depending on whether the time-reversal symmetry is broken \( \langle \Psi_{1(2)} \rangle \propto | \Psi_{2(1)} \rangle \) or not \( \langle \mathcal{K}| \Psi_{1(2)} \rangle \propto | \Psi_{1(2)} \rangle \). For each case, the symmetry-breaking GSs are constructed as

\[
| \Psi_{1,2} \rangle = (| \Phi_1 \rangle \pm i| \Phi_2 \rangle)/\sqrt{2} \quad (\mathcal{K}\text{-unbreaking case}),
| \Psi_{1,2} \rangle = (| \Phi_1 \rangle \pm | \Phi_2 \rangle)/\sqrt{2} \quad (\mathcal{K}\text{-breaking case}).
\]

Here the both possibilities have to be examined since,
due to the anti-unitarity 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 which distinguishes the symmetry-breaking GSs by comparing the RDMs $\rho^i_\Omega = \text{Tr}_\Omega \{ \Psi_i \} \langle \Psi_i \rangle$ ($i = 1, 2$), where $\Omega$ is an area in the system and $\Omega$ its complement. To quantify to what extent the two RDMs are different, we introduce a measure as

$$\text{diff}^1(\rho^1_\Omega, \rho^2_\Omega) = \max_{|O_\Omega| \leq 1} \left| \text{Tr}(O^1_\Omega \rho^1_\Omega) - \text{Tr}(O^2_\Omega \rho^2_\Omega) \right|, \quad (2)$$

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

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

$$\text{diff}^1(\rho^1_\Omega, \rho^2_\Omega) = \max_{|O_\Omega| \leq 1} \left| \sum_j \lambda_j | j \rangle O_\Omega | j \rangle \right| = \sum_j | \lambda_j |. \quad (3)$$

Here the maximization is done by the “optimal” order parameter:

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

where $\text{sgn} \lambda_j$ is the sign of $\lambda_j$ 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 K-unbreaking and K-breaking combinations in eq. (4). In the following, we denote the measure (2) for the K-unbreaking and 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

$$| \Psi^\text{Néel}_1 \rangle = \frac{1}{\sqrt{2}} (| \uparrow \downarrow \cdots + | \downarrow \uparrow \cdots \rangle), \quad (5)$$

$$| \Psi^\text{dimer}_1 \rangle = \frac{1}{\sqrt{2}} (| s_{12} \cdots s_{N-1,N} \pm | s_{23} \cdots s_{N,1} \rangle), \quad (6)$$

where $| s_{ij} \rangle$ denotes a singlet bond. For the Néel order, diff1 = 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 K-unbreaking GSs on $\{ 1 \}$, resulting in $O^{\text{opt}}_{\{ 1 \}} = 2S^\uparrow_1$. For the dimer order, on the other hand, both “diff1” and “diff2” are zero for $\{ 1 \}$ but we find diff1 = 3/2 > 0 for a 2-site area $\{ 1, 2 \}$. The resultant optimal order parameter (4) for this area is $O^{\text{opt}}_{\{ 1, 2 \}} = 2S^\uparrow_1 \cdot S^\downarrow_2 + 1/2$. 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 would be only able to calculate 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 finite-size effect is outside the scope of the present 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:

$$\mathcal{H} = \cos \theta \sum_i S_i \cdot S_j + \sin \theta \sum_i (P_i + P_i^{-1}), \quad (7)$$

where the 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 $\theta_c = \tan^{-1}(1/2) \approx 0.1476 \pi$ [4]; see Fig. 3a.

| Area $\Omega$ | $\theta = 0.12\pi$ | $\theta = 0.19\pi$ |
|-------------|-----------------|-----------------|
| $\{ 1 \}$   | 0.0000 0* 0* 0* | 0.0000 0* 0* 0* |
| $\{ 1, 2 \}$| 0.5698 0* 0.0029 0* | 0.5698 0* 0.0029 0* |
| $\{ 1, 1' \}$| 0.0000 0* 0* 0* | 0.0000 0* 0* 0* |
| $\{ 1, 2' \}$| 0.5698 0* 0.0029 0* | 0.5698 0* 0.0029 0* |
| $\{ 1, 2, 1' \}$| 0.5698 0.0267 0.0029 0.3340 | 0.5698 0.0267 0.0029 0.3340 |
| $\{ 1, 2, 3 \}$| 0.6579 0.0670 0.0033 0.2365 | 0.6579 0.0670 0.0033 0.2365 |
| $\{ 1, 2, 1', 2' \}$| 0.5698 0.0462 0.0029 0.5785 | 0.5698 0.0462 0.0029 0.5785 |

TABLE I: Values of “diff” for various areas in the 14 × 2 ladder. The points, $\theta = 0.12\pi$ and $0.19\pi$, 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.

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

| 1' | 2' | 3' | 4' | 5' | 6' |
|----|----|----|----|----|----|
| 1  | 2  | 3  | 4  | 5  | 6  |
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 \(\sigma\) the reflection with respect to a rung. We constructed symmetry-breaking GSs from these states and calculated “diff” for various areas; see Table II. 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 \(S_1 \cdot S_2\) and hence the optimal order parameter is \(O_{\{1, 2\}}^{(opt)} = 2S_1 \cdot S_2 + 1/2\). 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 \(\Delta \rho_{\{1, 2, 1'\}} \propto S_1 \cdot (S_2 \times S_1')\), and hence \(O_{\{1, 2, 1'\}}^{(opt)} = \frac{1}{3\sqrt{2}}S_1 \cdot (S_2 \times S_1')\). In 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), \(\theta\)-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 \(\theta_s\), confirming the phase transition between the two ordered phases. For \(\{1, 2, 1', 2'\}\), the values of “diff1” and “diff2” cross exactly at \(\theta_s\). For \(\{1, 2, 1'\}\), the crossing of “diff1” and “diff2” deviates from \(\theta_s\) but approaches it when increasing the system size. In general, such a crossing indicates a phase transition between ordered phases which cannot be distinguished by the GS quantum numbers.

**Application II** — We next consider a solvable QDM on the kagome lattice introduced recently [9] (for a review, see also section 5 of Ref. [8]), which is one of the microscopic models realizing a short-ranged (so-called \(Z_2\)) RVB liquid. This model also provides an example of a solvable Hamiltonian \(\hat{H}\) for a topological quantum-bit based on a QDM [8]. 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 \(\mathcal{C}\) 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 which flips the arrow on the site \(i\) of \(K\). Dimer movements can be represented as loop products of \(\tau^z\) operators. The Hamiltonian we consider is the sum of the loop operators around the hexagons \(h\) of \(K\): \(\mathcal{H} = -\sum_h \prod_{\alpha=1}^6 \tau^z(h, \alpha)\), where \(h, \alpha\) are the six sites of the hexagon \(h\).

If this model is defined on a surface with a *non-trivial topology* (cylinder, torus, etc.), arrow configurations in \(S\) can be grouped into topological sectors which 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 \(\Delta\) (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 \(\Delta\) to the right is even or odd. The spectrum can be determined separately in each sector. Using the standard Rokhsar-Kivelson argument [10], 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:

\[
|\mu\rangle = \frac{1}{\sqrt{|S|}} \sum_{a \in S} |a\rangle, \quad \mu = +, -.
\]

These two states are exactly degenerate and form a 2-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 \(\Omega\) is given as a set of bonds of \(H\). The RDM \(\rho_{\Omega} = \text{Tr}_\Omega |\Psi\rangle \langle \Psi|\) is defined by tracing out the degrees of
(b) Local area $\Omega$ on the cylinder. The cut $\Delta$ and the loop freedom (arrows) on $\bar{\Omega}$:

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

(9)

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

$$
\rho_\Omega = \sum_{\mu,\nu} \alpha_\mu \alpha_\nu^* M_{\Omega}^{\mu\nu}, \quad M_{\Omega}^{\mu\nu} = \text{Tr}_\Omega \langle \mu|\nu\rangle.
$$

(10)

First we assume that $\Omega$ is a (finite) local area; see Fig. (b). We prove the following relations:

$$
M_{\Omega}^{\mu\nu} = 0, \quad M_{\Omega}^{\mu\nu} = M_{\bar{\Omega}}^{\mu\nu},
$$

(11)

where the overbars represent the sign flip. To prove the first relation, we choose the cut $\Delta$ so as not to touch $\Omega$. Then the parity along $\Delta$ for an arrow configuration depends only on its part on $\Omega$. Let us consider the matrix element of $M_{\Omega}^{\mu\nu}$:

$$
\langle a_1|M_{\Omega}^{\mu\nu}|a_2\rangle = \sum_a \langle a_1, \bar{a}|+\rangle(-|a_2, \bar{a}\rangle).
$$

Since the two configurations, $(a_1, \bar{a})$ and $(a_2, \bar{a})$, have common parity, $\langle a_1, \bar{a}|+\rangle$ and $(-|a_2, \bar{a}\rangle$ cannot be non-zero at the same time and hence we obtain $M_{\Omega}^{\mu\nu} = 0$.

To prove the second relation in Eq. (11), we draw a loop $\Delta^*$ (passing along the bonds of $H$) encircling the cylinder so as not to touch the area $\Omega$. We introduce a loop operator along $\Delta^*$: $T_{\Delta^*} = \Pi_{i=1}^{n-\Delta^*} (i)$. This operator acts only on $\bar{\Omega}$ and maps $|\pm\rangle$ to $|\mp\rangle$, showing $M_{\Omega}^{\mu\nu} = \text{Tr}_\Omega (T_{\Delta^*}|\mu\rangle\langle\nu|T_{\Delta^*}^\dagger) = \text{Tr}_\Omega (|\mu\rangle\langle\nu|(T_{\Delta^*}^\dagger)^2) = M_{\bar{\Omega}}^{\mu\nu}$.

From Eqs. (10) and (11), we see that $\rho_\Omega$ 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, this shows the stability of quantum information against external noises (coupling locally to dimers).

The situation is different if $\Omega$ has a non-trivial 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 $\Delta$ inside $\Omega$. Then the parity along $\Delta$ can be expressed as the operator acting on $\bar{\Omega}$ and distinguishes the different topological sectors. It can be considered as a non-local order parameter distinguishing $|\pm\rangle$ and $|\mp\rangle$. Similarly, in case B, two states $(|\pm\rangle \pm |\mp\rangle)/\sqrt{2}$ are distinguished by the loop operator $T_{\Delta^*}$ with $\Delta^*$ defined inside $\Omega$.

We have shown that the GSs of this QDM cannot be distinguished by any local operator but by non-local operators defined on areas with non-trivial topologies. We comment that a similar result has been shown without using RDMs by Ioffe and Feigel’man 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 which 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. [6] 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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[12] An order parameter is local, if it acts on a finite area, even when the size of the entire system is taken to infinity.
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