Reduced density matrices and topological order in a quantum dimer model

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Abstract
Resonating valence bond (RVB) liquids in two dimensions are believed to exhibit topological order and to admit no local order parameter of any kind. This is a defining property of 'liquids', but it has been confirmed explicitly only in a few exactly solvable models. In this paper, we investigate the quantum dimer model on the triangular lattice. This possesses an RVB-type liquid phase, however, for which the absence of a local order parameter has not been proved. We examine the question numerically with a measure based on reduced density matrices. We find a scaling of the measure which strongly supports the absence of any local order parameter.

1. Introduction

The existence of short-ranged resonating valence bond (RVB) liquids has been proposed in several two-dimensional quantum spin models [1]. These liquids exhibit no kind of simple order, but the ground states (GS) are degenerate if the lattice is put on a surface with a non-trivial topology (cylinder, torus, etc). It is (widely) believed that such degeneracy has a purely topological origin and is not ascribed to spontaneous symmetry breaking in terms of any local order parameter. This topological nature has been rigorously confirmed in a few exactly solvable models [2, 3], but proving this property in more general cases is a challenging issue.

In this paper, we address this issue by formulating the problem in terms of reduced density matrices (RDM), as we proposed in [3]. In this formulation, we examine the RDMs of the degenerate GSs for various sub-areas of the system and search for an operator distinguishing the degenerate GSs, which means that it can be used as an order parameter. We define a convenient measure for this purpose, which is non-zero for an area where an order parameter can be defined. In conventional orders, the measure is non-zero on some finite local area, which indicates the existence of an order parameter on that area. In RVB liquids, in contrast,

it is expected that the measure is zero (in the thermodynamic limit) on any local area, thereby verifying topological order.

With this formulation, we analyse the quantum dimer model (QDM) on the triangular lattice, which is one of the simplest microscopic models realizing an RVB liquid [4]. We show numerically that the dimer liquid in this model cannot be characterized by any local order parameter.

2. Formulation

2.1. General case

We formulate a method to detect an order parameter starting from a general setting. Let q be the degeneracy of the GSs and $|\Phi_i\rangle$ ($i = 1, \ldots, q$) be the orthonormal GSs. For a state $|\Psi\rangle$ in the ground-state subspace, we define its RDM on an area Ω by tracing out the degrees of freedom outside Ω: $\rho_\Omega \equiv \mathrm{Tr}_{\bar\Omega} |\Psi\rangle\langle\Psi|$, where $\bar\Omega$ is the complement of Ω. We also introduce as a reference the RDM averaged over the ground-state subspace: $\rho_\Omega^{\mathrm{ref}} \equiv \frac{1}{q} \mathrm{Tr}_{\bar\Omega} \sum_{i=1}^{q} |\Phi_i\rangle\langle\Phi_i|$. Note that $\rho_\Omega^{\mathrm{ref}}$ is independent of the choice of the basis $\{|\Phi_i\rangle\}$ of the ground-state subspace. An order parameter can be defined on Ω if and only if there exists $|\Psi\rangle$ such that $\rho_\Omega \neq \rho_\Omega^{\mathrm{ref}}$.

To quantify to what extent RDMs are distinguishable, we introduce a measure D_Ω as follows. We first define a measure of difference between two RDMs as [3]

$$\mathrm{diff}(\rho_\Omega, \rho_\Omega^{\mathrm{ref}}) \equiv \max_{|\mathcal{O}_\Omega| \leqslant 1} \left| \mathrm{Tr}_\Omega(\mathcal{O}_\Omega \rho_\Omega) - \mathrm{Tr}_\Omega(\mathcal{O}_\Omega \rho_\Omega^{\mathrm{ref}}) \right|, \tag{1}$$

where $\mathcal{O}_\Omega$ is a (variational) Hermitian operator on Ω whose norm is less than unity, i.e. $|\langle\psi|\mathcal{O}_\Omega|\psi\rangle| \leqslant 1$ for any normalized vector $|\psi\rangle$. Using the eigenvalues $\{\lambda_j\}$ of $\rho_\Omega - \rho_\Omega^{\mathrm{ref}}$, this can be simplified as $\mathrm{diff}(\rho_\Omega, \rho_\Omega^{\mathrm{ref}}) = \sum_j |\lambda_j|$. We define D_Ω by maximizing $\mathrm{diff}(\rho_\Omega, \rho_\Omega^{\mathrm{ref}})$ over the choice of a GS $|\Psi\rangle$:

$$D_\Omega \equiv \max_{|\Psi\rangle} \mathrm{diff}(\rho_\Omega, \rho_\Omega^{\mathrm{ref}}). \tag{2}$$

The value of D_Ω in the thermodynamic limit tells us whether an order parameter can be defined on Ω. The measure D_Ω has the following useful properties: (a) normalization to a definite range $0 \leqslant D_\Omega \leqslant 2 - 2/q$; (b) monotonicity—if an area Λ completely contains an area Ω, we have $D_\Omega \leqslant D_\Lambda$.

How to calculate D_Ω is not clear from the definition. In the case of QDMs, a simple formula is available, which we derive in the next subsection. However, for the completeness of the method, here we briefly describe a general algorithm called *iterative maximization*. The difficulty in calculating D_Ω resides in the double maximizations in equations (1) and (2), but we notice that each maximization is possible if either $\mathcal{O}_\Omega$ or $|\Psi\rangle$ is fixed. The idea is to perform these two kinds of maximizations alternately, starting from a random vector $|\Psi\rangle$. This would lead at least to a local maximum in the space of $\mathcal{O}_\Omega$ and $|\Psi\rangle$. Starting from various random vectors, we would obtain the global maximum D_Ω. This method has the potential to handle a wide range of problems.

2.2. Case of quantum Dimer models

We limit the setting to the case of gapped dimer liquids in QDMs on two-dimensional lattices, where further argument is possible. The gapped dimer liquids have been found in several QDMs [4, 6] and related models [2, 7]. However, except for the special cases [2, 3, 6] where the correlation length is strictly zero, it is difficult to prove the absence of any local order parameter. This motivates us to study more general cases.

Let S be the set of all the dimer coverings of the lattice. If the lattice has a non-trivial topology, S can be grouped into topological sectors which are not mixed by any local operation. We concentrate on the case of the torus in the following. We draw two incontractible loops, Δ_1 and Δ_2, which pass through the bonds and wind the torus in x and y directions, respectively. We classify S into four topological sectors S^p with $p = ++, +-, -+, --$, depending on the parity of the number of dimers crossing Δ_1 and Δ_2. In a gapped dimer liquid, the lowest-energy states $|\Phi_p\rangle$ in different topological sectors S^p become degenerate in the thermodynamic limit. We employ $\{|\Phi_p\rangle\}$ as the basis of the ground-state subspace.

To define RDMs for QDMs, we must specify the local degrees of freedom of the models. To this end, we assign an Ising variable σ_k to each bond k of the lattice as in [8] and identify the presence/absence of a dimer on the bond as $\sigma_k = +1$ and -1, respectively. Any physical configuration $\{\sigma_k\}$ must satisfy the hard-core constraints: for each site of the lattice, there must be exactly one bond with $\sigma_k = 1$ emanating from it. An area Ω is defined as a set of bonds. We define the matrix element of the RDM of a GS $|\Psi\rangle$ as

$$\langle c_1|\rho_\Omega|c_2\rangle = \sum_{\bar{c}}\langle c_1, \bar{c}|\Psi\rangle\langle\Psi|c_2, \bar{c}\rangle, \tag{3}$$

where c_1 and c_2 are dimer configurations on Ω and the sum is over all the dimer configurations $\bar{c}$ on $\bar{\Omega}$. Note that we set $\langle c, \bar{c}|\Psi\rangle = 0$ if $(c, \bar{c})$ is an unphysical configuration (violating the hard-core constraint).

We proceed to the evaluation of D_Ω. We first assume that the area Ω is topologically non-trivial, i.e. Ω encircles the torus. Without loss of generality, we assume that Ω contains Δ_1. Let us consider the following trial GS and trial operator:

$$|\Psi^{(\text{trial})}\rangle = |\Phi_{++}\rangle, \qquad \mathcal{O}_\Omega^{(\text{trial})} = \sum_c |c\rangle P(c)\langle c|,$$

where, in the second equation, c runs over all the dimer configurations on Ω and $P(c)$ is its parity along Δ_1. These give a lower bound of D_Ω:

$$D_\Omega \geqslant |\operatorname{Tr}_\Omega \mathcal{O}_\Omega^{(\text{trial})}(\operatorname{Tr}_{\bar{\Omega}}|\Psi^{(\text{trial})}\rangle\langle\Psi^{(\text{trial})}| - \rho_\Omega^{\text{ref}})| = 1.$$

Thus the value of D_Ω is consistent with the existence of a non-local order parameter.

We next assume that Ω is a (finite) local area. In this case, we can prove the following relation:

$$\operatorname{Tr}_{\bar{\Omega}}|\Phi_p\rangle\langle\Phi_{p'}| = 0 \qquad (p \neq p'). \tag{4}$$

To prove this relation, we explicitly express the matrix element of the left-hand side:

$$\langle c_1|\left(\operatorname{Tr}_{\bar{\Omega}}|\Phi_p\rangle\langle\Phi_{p'}|\right)|c_2\rangle = \sum_{\bar{c}}\langle c_1, \bar{c}|\Phi_p\rangle\langle\Phi_{p'}|c_2, \bar{c}\rangle.$$

Since Ω is local, we can choose Δ_1 and Δ_2 so as not to touch Ω. Then the dimer coverings $(c_1, \bar{c})$ and $(c_2, \bar{c})$ always belong to a common topological sector, and therefore $\langle c_1, \bar{c}|\Phi_p\rangle$ and $\langle\Phi_{p'}|c_2, \bar{c}\rangle$ cannot become non-zero at the same time. Hence we obtain equation (4). Using equation (4), we can derive a simpler expression for D_Ω:

$$D_\Omega = \max_p \operatorname{diff}(\rho_\Omega^p, \rho_\Omega^{\text{ref}}), \qquad \text{with } \rho_\Omega^p \equiv \operatorname{Tr}_{\bar{\Omega}}|\Phi_p\rangle\langle\Phi_p|. \tag{5}$$

This is computable numerically and is employed in the calculation shown below.

3. Numerical result

We consider the QDM on the triangular lattice. The Hamiltonian reads [4]:

$$H = \sum_{\text{rhombi}}\left[-t\left(|{/\!\!/}\rangle\langle{\scriptstyle\smile\,\smile}| + \text{h.c.}\right) + v\left(|{\scriptstyle\smile\,\smile}\rangle\langle{\scriptstyle\smile\,\smile}| + |{/\!\!/}\rangle\langle{/\!\!/}|\right)\right]. \tag{6}$$
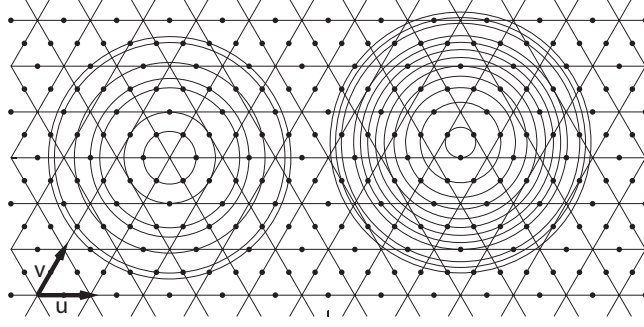
Figure 1. Circular areas centred around a site (left) or an interior of a triangle (right).
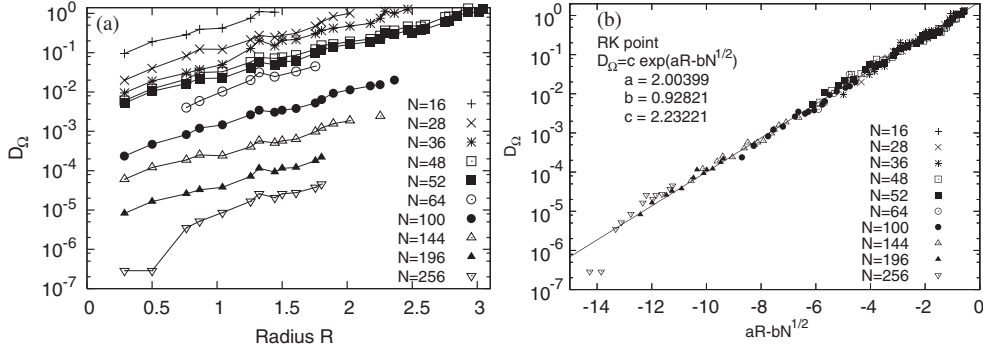

Figure 2. The result for the RK wavefunction: (a) the value of D_Ω as a function of the radius R for different system sizes N; (b) fitting of the data using an exponential function $D_\Omega \approx ce^{aR-b\sqrt{N}}$.

At the Rokhsar–Kivelson (RK) point ($v = t$), the GS in each sector is exactly the equal-amplitude superposition of all the dimer coverings belonging to that sector [4, 5]:

$$|\Phi_p\rangle = \frac{1}{\sqrt{|S^p|}} \sum_{C \in S^p} |C\rangle. \tag{7}$$

It has been shown numerically that the degeneracy of the GSs and the exponential decay of the dimer–dimer correlation at the RK point persist up to some range in the parameter space, forming a dimer liquid phase in $0.7 \lesssim v/t \leqslant 1$ [4, 9–11].

We first calculated D_Ω numerically for the RK wavefunction, equation (7), through the direct enumeration of dimer coverings (up to $N = 52$) or the evaluation of Pfaffians of Kasteleyn matrices [12] (up to $N = 256$). The former method is suited for large areas, while the latter can handle large systems. The lattice is put on the torus and is defined by two vectors, T_1 and T_2, specifying the periodicity. We require that the lattice is symmetric under the $2\pi/3$ rotation, choosing $T_1 = lu + mv$ and $T_2 = -mu + (l + m)v$, where l and m are integers and u and v are unit vectors, as shown in figure 1. The total number of sites is given by $N = l^2 + lm + m^2$. As the choice of Ω, we define circular areas in the following way: we draw a circle centred around a site or an interior of a triangle and regard every bond whose midpoint is in the circle as an element of the area (see figure 1). The values of D_Ω for circular areas are plotted versus the radius R in figure 2(a). Though D_Ω tends to increase as a function of R, it remains small if R is sufficiently smaller than the linear system size $\sqrt{N}$. It appears that an exponential dependence $D_\Omega \approx ce^{aR-b\sqrt{N}}$ fits the data relatively
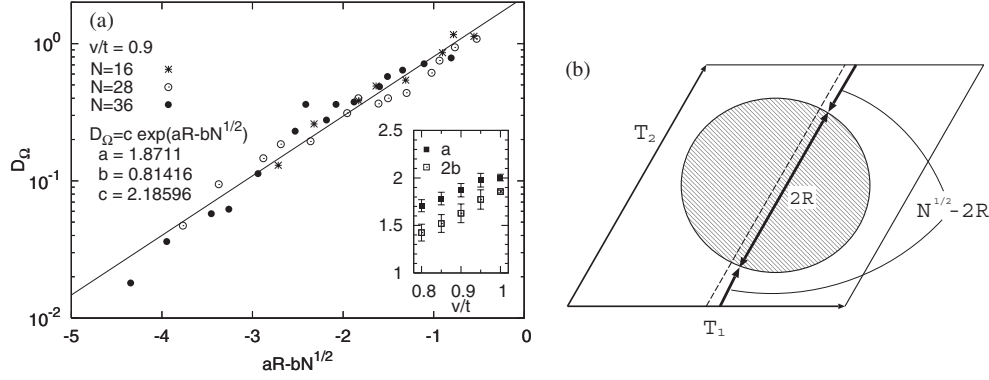
Figure 3. (a) Main panel: fitting of the data of D_Ω for $v/t = 0.9$. Inset: obtained fitting parameters a, b for different values of v/t in the dimer liquid phase. (b) A loop (broken line) encircling the torus and the area Ω. Periodic boundary conditions are imposed along T_1 and T_2. Part of the loop with a length of $\sqrt{N} - 2R$ is not covered by Ω.

well, as can be seen in figure 2(b). We also performed a calculation for $v/t < 1$ by obtaining GSs by exact diagonalization. We fit the data in the same way and the resultant parameters a and b are shown in the inset of figure 3(a). We observe that the relation $a \approx 2b$ holds approximately in the dimer liquid phase. This indicates that the finite-size effect in D_Ω enters through $\sqrt{N} - 2R$. To interpret this, let us consider a loop encircling the torus and passing through Ω; see figure 3(b). Some part of a loop is not covered by Ω and the minimal length of the part is $\sqrt{N} - 2R$. The lack of this part makes the distinction of sectors obscure, hence the exponential reduction in D_Ω. Our result shows explicitly the topological nature of the liquid, since D_Ω goes to zero exponentially with $N \to \infty$ *for any fixed R*. This not only excludes local order parameters which are diagonal in the dimer basis (and amenable to exact calculations in the $N \to \infty$ limit [11]), but any operator, possibly non-diagonal, too. The parameter b is naturally interpreted as the inverse of a correlation length, and the value we obtained at the RK point is close to $\xi_A^{-1} \approx 0.83 \pm 0.12i\pi$ and $\xi_B^{-1} \approx 0.76$ obtained by [11], where A refers to the direction along a bond and B refers to the direction perpendicular to it.

4. Conclusion

We formulated a method to detect the existence of an order parameter using reduced density matrices. We applied the method numerically to the liquid phase of the QDM on the triangular lattice. The measure D_Ω that we defined contrasts local areas with non-local areas: $D_\Omega \to 0$ with $N \to \infty$ on local areas, while $D_\Omega \geqslant 1$ on non-local areas. The data of D_Ω is fitted well by an exponential function, which can be interpreted from the topological picture. Our result explicitly verifies topological order in this system.

Acknowledgments

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