Generic phase diagram of quantum dimer model on square lattice

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Constraint is an important property in low-energy physics, but it also bring a lot of difficulties for numeric calculation. The quantum dimer model is a low-energy description of many spin models, but its phase diagram is still controversial, even on the square lattice. In this article, we focus on the square lattice quantum dimer model and give a unified conclusion about its phase diagram which reconciles conflicting results given in the literature. With our newly developed sweeping cluster method, we studied the phase diagram of the almost full parameter space by introducing the definition of pair correlation function and other supporting evidence to distinguish the mixed phase from the columnar phase with high precision. In particular, we find that the ground state corresponds to the mixed phase for a vast parameter region.

Introduction. Constraints are a common theme in modern many-body physics when there is a particularly large energy scale in the Hamiltonian. In low-energy physics, systems often have constraints. In mathematics, we usually use gauge field theory to deal with them. However, many constraints are difficult to deal with numerically, which directly delays our research and understanding of some many-body systems such as quantum dimer models (QDMs). QDMs featured by strong geometric restrictions are effective low energy descriptions of many quantum spin systems. It was first introduced by Rokhsar and Kivelson (RK) to study the physics of the short-range resonating valence bond (RVB) state which is probably related to high-$T_c$ cuprates. QDMs provide particularly simple examples to realize topological phases, such as a two-dimensional gapped phase with $\mathbb{Z}_2$ topological order, and a three-dimensional Coulomb phase described by an emergent $U(1)$ symmetry. Recently, a QDM for the metallic state of the hole-doped cuprates was also proposed to describe the mysterious pseudogap state at low hole density. At the same time, constraints also hinder the application of algorithms, phase diagrams of quantum dimer models are still controversial, even on square lattice.

The QDM Hamiltonian on square lattice can be written as

$$H = -\sum_{\text{plaq}} \left( \mathbb{I} \otimes H_c \right) + V \sum_{\text{plaq}} \left( \mathbb{I} \otimes \mathbb{I} + \mathbb{I} \otimes \mathbb{m} \right),$$

where the summations are taken over all elementary plaquettes of the lattice. A dimer represents an $SU(2)$ singlet bond between two spins located at its endpoints, and the kinetic term describes a resonance between the two dimerizations of a plaquette. This seemingly simple Hamiltonian contains a strong constraints which requires

\[ |GS\rangle = \sum_{\text{plaq}} A_C |C\rangle \]

where $A_C = A_{C'}$ for $C$ and $C'$ in the same winding sector. However, the model, eq. (1), cannot be solved exactly for other parameter values, and there are still disputes about its phase diagram, as illustrated in Fig. 1.

For $V = -\infty$ the Hamiltonian strongly favors configurations with as many parallel dimers as possible. This is achieved by the ground states such as shown in Fig. 1 bottom left. It has been argued that this state extends all the way up to the RK point, phase diagram 3 in Fig. 1 where the ground state becomes the staggered state. The same phase diagram is also supported by Metropolis Monte Carlo simulations on height model equivalents of the square lattice QDM and

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the frustrated transverse field Ising model which is equal to a parameter point \((V = 0)\) of QDM \([13]\).

The projection Monte Carlo method does obey the geometric constraints, but it is difficult to work in the parameter interval away from the RK point \((V = 1)\) \([19]\). Through this method, some scholars have concluded that due to quantum fluctuations, there will be a phase that breaks translational symmetry both along the x- and y-axes near the RK point, a rotationally symmetric plaquette state \([11, 12, 20]\), shown as the 1st phase diagram of Fig. 1. On the other hand, the square lattice quantum dimer model is closely related to the \((2 + 1)\)-dimensional \(U(1)\) quantum link model \([21, 23]\). In particular, there are two distinct confining phases (analogous to columnar and plaquette phases in the quantum dimer model) with different discrete symmetry breaking patterns, separated by a weak first-order phase transition that mimics several features of deconfined quantum critical points \([24–26]\).

Another candidate ground state, the mixed state, which breaks rotational symmetry as well as translational symmetry both along the x- and y-axis can be thought of as a mixture of the plaquette and the columnar state. It looks similar to the plaquette state. However, the strengths in the x and y directions of the same plaquette are different \([13]\). This phase is shown as the 3rd one of Fig. 1 bottom.

In this paper, we are committed to solving the phase diagram dispute and giving a result that reconciles all contradictions. Using our newly developed exact method – sweeping cluster algorithm \([27]\), we calculated the phase diagram of the square lattice QDM as the 4th one of Fig. 1.

**Mixed phase.** There were strong evidences that the plaquette phase do not exist on square lattice \([13]\). So the first question is whether there is a mixed phase or only columnar phase. Selecting \(V = 0.5\), we carefully studied the ground state. Different states can be distinguished by different distributions of VBS order parameter as Fig. 1(a) shown. The yellow points represent the columnar state with 4-fold degeneracy. The black ones represent the plaquette state with 4-fold degeneracy. The white ones between black and yellow points indicate mixed state which has eight-fold degeneracy. It is worth noting that the white points are not necessarily in the exact middle of black and yellow. It can move in the region depending on the degree of mixing. The VBS order parameter on complex plane above is defined as \([17]\):

\[
\Psi_{\text{col}} = \frac{1}{L^2} \sum_{\mathbf{r}} \left\{ (-1)^{s_x} \left[ n(\mathbf{r} + \frac{x}{2}) - n(\mathbf{r} - \frac{x}{2}) \right] + i(-1)^{s_y} \left[ n(\mathbf{r} + \frac{y}{2}) - n(\mathbf{r} - \frac{y}{2}) \right] \right\},
\]

where \(x\) and \(y\) are unit vectors and \(L\) is the linear system size. The dimer number operator \(n(\mathbf{r} + \mathbf{e}/2)\) is 1 if the site at \(\mathbf{r}\) and its nearest neighbor at \(\mathbf{r} + \mathbf{e}/2\) form a dimer, and zero otherwise.

The VBS order parameter distribution Fig. 2(b) peaks at the location of the yellow points in Fig. 2(a). This has been taken as the main evidence for the columnar state in Ref. \([14, 18]\). However, when we extract one of the peaks and plot its distribution as a function of the order parameter angle \(\theta\), we observe that the distribution has a flat maximum which can equally well be interpreted as a combination of two peaks centered on \(\pm \theta_0\) to the sides of the yellow point, as we have fitted in Fig. 2(c). Thus it is possible to interpret the flat maxima at the “columnar” points of the order parameter distributions.

![Figure 2](image-url)

**FIG. 2.** (a) VBS order parameter distributions of the various candidate phases: columnar (yellow points), plaquette (black points) and mixed (white points). (b) VBS order parameter distributions of different \(V, T = 0.01, L = 32\). (c) Blue dashed is the distribution plan of a certain peak of \(V = 0.5\), radial integration only the angle left. The data collection points of one peak in (b) and (c) is about 80,000. Red solid line is the distribution of angle without radial integration, i.e., fix a certain radius which go through the peak of (b). Gray dashed is the two peaks fitting for the blue angular distribution. (d) The average dimer occupation near the center of an \(L = 64\) lattice for \(V = 0.5\). Red/blue color represents that the dimer occupation is larger/smaller than 1/4 (the average number when no long range order exists), indicating the tendency to find one/no dimer at that location. We choose the parameters as \(V = 0.5, T = 0.01\).
as being instead two mixed-phase peaks. What’s more, if we fix a certain radius, the distribution of angle looks more like two peaks as the red line of Fig. 2(c). The position of two peaks is very close to the fitting ones.

It is hard to distinguish different states by average configurations directly since all three states (columnar, plaquette, mixed) are degenerated. To remove the degeneracy we have to act with a projection operator on the sampling configurations of Monte Carlo data. Specifically we define an operator $(\mathbb{I})_n$ which defines a projection operator onto parallel horizontal dimers on the $n$th plaquette of the square lattice. As shown in Fig. 2(d), average value of projected configurations is clearly not a columnar phase.

To further investigate vaster region and much stronger evidence, we also measure dimer pair correlation functions. We define the pair dimer operator on plaquette $p$ as

\[ D_{\mathbb{I},p} = \mathbb{I}_{p} \mathbb{I}, \quad D_{\mathbb{II},p} = \mathbb{I}_{p} \mathbb{I}, \]

and the pair correlation function $C_{ij,|p-q|}$ between $D_{i,p}$ and $D_{j,q}$ as:

\[ C_{ij,|p-q|} = \frac{\langle D_{i,p}D_{j,q} \rangle - \langle D_{i,p}\rangle\langle D_{j,q}\rangle}{\langle D_{i,p}\rangle - \langle D_{i,p}\rangle^2} \]

where $i, j = \mathbb{I}, \mathbb{II}$ and $|p-q|$ means the distance. We focus on $\Delta C_{\mathbb{II}}$ which is the difference of the two largest distance correlations, i.e. $p = (0,0)$, $q = (L/2, L/2)$ and $p = (0,0)$, $(L/2+1, L/2)$. Similarly, $\Delta C_{\mathbb{II}}$ is the difference of the two largest distance correlations of $p = (0,0)$, $q = (L/2, L/2)$ and $p = (0,0)$, $q = (L/2, L/2+1)$. At $V = 0.5$ and $T = 0.01$, we plot those for different system sizes in Fig. 3.

If there is a columnar phase, $\Delta C_{\mathbb{II}}$ should remain finite as $L \to \infty$ while $\Delta C_{\mathbb{II}}$ should fall to 0. For a plaquette phase $\Delta C_{\mathbb{II}} = \Delta C_{\mathbb{II}}$ while a mixed phase is characterized by finite but different values of $\Delta C_{\mathbb{II}}$ and $\Delta C_{\mathbb{II}}$ in the same limit. As shown in Fig. 3(a), our results taken from system sizes up to $L = 64$ indicate a mixed phase. We can conclude here for $V = 0.5, 0, -0.5$ that there are substantial mixed phase correlations.

Furthermore, as $V = 0$ is far away from the RK-point, we also measured the structure factor through different correlation function as shown in Fig. 3(b). Using single dimer correlation function $C_{\mathbb{II}}$ and $C_{\mathbb{III}}$, we got the structure in k-space as (i) and (ii). It looks the symmetry is as same as columnar phase because single dimer correlation function can not separate two mixed states which are mirror symmetric along a dimer. It is very different if we use pair correlation function $C_{\mathbb{II}}$ and $C_{\mathbb{II}}$ to measure the structure, as shown in (iii) and (iv). That’s clearly a structure of mixed phase in k-space.

Both $\Delta C_{\mathbb{II}}/\Delta C_{\mathbb{II}}$ and $\theta_0$ are features of mixed state. They are positively correlated under various $V$ as inset of Fig. 3(c). This is consistent with our starting point, i.e. the peak for columnar state is made up by two peaks for columnar state. What’s more, both $\Delta C_{\mathbb{II}}/\Delta C_{\mathbb{II}}$ and

\[\text{FIG. 3. (color online).} \text{ (a) The difference of longest distance pair dimer correlations $\Delta C_{\mathbb{II}}$ (red) and $\Delta C_{\mathbb{II}}$ (blue). (b) The structure factor of different dimer correlation functions under size $L = 56$, temperature $T = 0.01$ and parameter $V = 0$: (i) Single dimer correlation function $C_{\mathbb{II}}$. (ii) Single dimer correlation function $C_{\mathbb{II}}$. (iii) Pair correlation function $C_{\mathbb{II}}$. (iv) Pair correlation function $C_{\mathbb{II}}$. (c) The relationship of the distance of two mixed state peaks $\theta_0$ and $V$ under certain size $L = 32$ and temperature $T = 0.01$. Inset: The relation for various $V$ ($V = -0.5, 0, 0.5, 0.9$) between distance of two mixed state peaks $\theta_0$ and $V$ under certain size $L = 32$ and temperature $T = 0.01$.}\]
\( \theta_0 \) do not decay rapidly when \( V < 0 \) from this figure. This means that the mixed state may extend to an area of small \( V \). Since the distributions of VBS order parameter can only be obtained in finite sizes, further study is needed.

\[
\Delta \ln \langle \phi_0 \rangle^2 / \Delta \ln \langle \phi \rangle^2 = 0. \quad \text{It becomes back to “pair update” which means operators flip only when they are face to face(in the same plaquette). “Pair update” works well on square lattice, see the appendix for related explanations. It can be switched between the columnar state and the plaquette state. We set the initial state of QMC to the columnar state and performed “pair update” to see whether columnar state becomes into mixed phase. In fact, it is a quantum perturbation on columnar state by numerical method. Then we did a finite \( V \) scaling as Fig. 4(a). The \( \Delta \ln \langle \phi_0 \rangle^2 / \Delta \ln \langle \phi \rangle^2 \) which indicates the characteristics of the mixed state, is always exist and power law dependencies with \( 1/(1-V) \). This means that as long as there is a quantum fluctuation term, the system is always in a mixed state, even if it is very small. Since these proofs, we could have a clear cognition about the phase diagram of QDM on square lattice. At classical limit, columnar phase is the ground state. When we add kinetic term into the Hamiltonian, it becomes a mixture of columnar state and plaquette state. After \( V > 1 \) (RK point), the conclusion remains that the system enters a staggered state.

Qualitative analysis.- We try to understand the emergence of mixed states through a simple qualitative analysis. When \( V = -\infty \), we can make further corrections in the context of a columnar state as Fig. 4(b). The solid line indicates where the dimer is located, that is, the initial state is the columnar state. Suppose there are a lot of plaquettes that need to be flipped for high-order correction. How is energy optimized? If the \( a \) plaquette is rotated, a pair of dimers will be moved from the solid line position to the dotted line position. Then we can rotate the \( d \) plaquette because it has only one dimer now. We can rotate the \( g \) plaquette. One might ask why not flip the plaquette which is above \( g \). However, there will leave a single dimer on \( g \), which costs energy. This effect can be transmitted, so that the plaquettes favor to be flipped as \( i, i+2, i+4, i+6... \). Now we can choose one plaquette from \( c, f \) and \( i \) to rotate it. It is not difficult to find that the energy after flipping \( c \) and \( i \) is better than flipping \( f \) because they will have an optimization of potential energy \( V \) with \( a \) and \( g \). Then if we treat \( c \) and \( i \) as new \( a \) and \( g \), this effect also can be transmitted. So the translational symmetry breaks both along the x- and y-axis. Because we understand this physical image at \( V = -\infty \), the optimization of \( V \) is very important, so it is conceivable that the configuration of the mixed state is best for energy.

Phase diagram.- Our second question is where is the boundary of the mixed state, i.e., what is the entire phase diagram? Based on field theory analysis combined with exact diagonalization method, recent studies have shown that there should be no phase transition points from the classical limit (\( V = -\infty \)) to the RK point [14, 15]. A similar trend can also be seen in Fig. 4(c), the distance between two peaks of the mixed state also tends to a non-zero finite value though this is a result of finite size. In addition, we also measured difference of pair correlation function at \( V = -0.5 \) and got the similar result that there is still mixed phase, as Fig. 4(a).

Which phase is the system in when \( V \) is far smaller than \(-0.5 \)? When \( V \) is less than \(-1 \), for convenience, we use sweeping cluster method and take the constant \( C + V = 0 \). It becomes back to “pair update” which means operators flip only when they are face to face(in the same plaquette). “Pair update” works well on square lattice, see the appendix for related explanations. It can be switched between the columnar state and the plaquette state. We set the initial state of QMC to the columnar state and performed “pair update” to see whether columnar state becomes into mixed phase. In fact, it is a quantum perturbation on columnar state by numerical method. Then we did a finite \( V \) scaling as Fig. 4(a). The \( \Delta \ln \langle \phi_0 \rangle^2 / \Delta \ln \langle \phi \rangle^2 \) which indicates the characteristics of the mixed state, is always exist and power law dependencies with \( 1/(1-V) \). This means that as long as there is a quantum fluctuation term, the system is always in a mixed state, even if it is very small. Since these proofs, we could have a clear cognition about the phase diagram of QDM on square lattice. At classical limit, columnar phase is the ground state. When we add kinetic term into the Hamiltonian, it becomes a mixture of columnar state and plaquette state. After \( V > 1 \) (RK point), the conclusion remains that the system enters a staggered state.

Conclusions and Outlook.- We focus on reconciling the contradictions between several articles and give a unified conclusion about phase diagrams on square lattice quantum dimer model. As described in the paper by D. Banerjee et al. [14, 15], we also support that there is no phase transition point in the interval of \( V < 1 \). The difference is that we feel the main evidence of columnar state needs further explanation and verification. Thus we give strong evidences to support the conclusion that the mixed state exists in the article by A. Ralko et al. [13]. For the zero-temperature phase diagram of the square
lattice QDM, we give a new answer. We believe that the columnar state exists only at the classical limit of quantum dimer model. After the quantum kinetic term is added, the system enters a mixed phase, even if the quantum term is very weak. Furthermore, we will study the finite temperature phase diagram of QDM.

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Peak fitting of the VBS order distribution

This appendix will give a detailed description on the approach of distinguishing the peaks from the 2D distribution of VBS order parameter (Fig. 2).

The points we obtained are initially discretely distributed on grid points (4m, 4n). To obtain a continuous angular distribution, certain kinds of loyal smoothing and continuation are necessary.

We first carry out an image smoothing with radius σ to reduce the noise:

\[ \tilde{N}_{mn} = C \sum_{m' n'} N_{m'n'} \exp \left( \frac{(m' - m)^2 + (n' - n)^2}{2\sigma^2} \right). \quad (6) \]

We choose \( \sigma = \sqrt{3} \) because smoothing with this radius can make the image smooth enough without flattening the peaks, shown in Fig. 2(b). The angular distributions for various \( \sigma \) are shown in Fig. 2(c). We can see that \( \sigma^2 = 3 \) is the most satisfying.

The continuous 2D distribution \( \varphi(x, y) \) is obtained through a linear interpolation from the discrete distribution at the grid points \( \tilde{N}_{mn} \). After integrating out the radial part, we get the continuous angular distribution

\[ \varphi(\theta) = \int rdr \varphi(r, \theta) \quad (7) \]

The peaks from the angular distribution don’t follow the Gauss exp(−A/r²) type very well, so we use \exp(−A/rα) to fit our peaks, where \( \alpha \) is a tunable parameter. We carry out a four-parameter fitting

\[ \varphi(\theta) = C \left( e^{-A(\theta - \theta_0)^\alpha} + e^{-A(\theta + \theta_0)^\alpha} \right) \quad (8) \]

If \( \theta_0 = 0 \), then the distribution is single-peaked, and the system is in columnar state. If \( \theta_0 \neq 0 \), the system is in mixed state. The fitting of \( V = 0.9 \) data will have to add a constant term because of the influence of the orderless phase at RK point.

We carried out fittings for \( V = -0.5, 0, 0.5 \) and 0.9, shown in Fig. 7. We find that the ratio of distance of peaks to \( \Delta C \), \( \Delta C \) being proportional.
FIG. 5. (color online). (a)(b) The 2D distribution of VBS order parameter (a) before and (b) after an image smoothing; (c) The angular distribution for various smoothing radius $\sigma$; (d)–(g) The peak fittings of the angular distribution for (d) $V = -0.5$, (e) $V = 0$, (f) $V = 0.5$ and (g) $V = 0.9$.

FIG. 6. (color online). (a) The relationship of $\Delta C$ and size $1/L$ for different $V$ at $T=0.01$. (b) The relationship of $\Delta C$ and size $1/L$ for different $V$ at $T=0.01$.

**Sweeping cluster algorithm for $V < -1$ region**

In sweeping cluster method [27], we write the QDM Hamiltonian in terms of plaquette operators $H_p$, $H = -\sum_{p=1}^{N_p} H_p$, where $p$ labels a specific plaquette on the lattice. The plaquette operators are further decomposed into two operators: $H_p = H_{1,p} + H_{2,p}$, where $H_{1,p}$ is diagonal and $H_{2,p}$ is off-diagonal:

$$H_{1,p} = -V \left( \mathbb{1} \langle \mathbb{1} \rangle + \mathbb{1} \langle \mathbb{1} \rangle \right) + V + C,$$

$$H_{2,p} = \left( \mathbb{1} \langle \mathbb{1} \rangle + \mathbb{1} \langle \mathbb{1} \rangle \right).$$

We have subtracted a constant $N_p(V+C)$ from the QDM Hamiltonian, which should be kept in mind when calculating the energy. We do this because the constant $V + C$ makes all matrix elements of $H_{1,p}$ positive provided $C > \max(-V,0)$.

We choose $C = -V$ when $V < -1$ for simplicity. Although this will lose some of the updated vertices and make the update not ergodic enough, between the two alternative states (columnar and mixed), this update can be fully migrating. The sweeping cluster algorithm works in region $(-\infty,0)$ when we choose $C = -V$ and works in $(-1,\infty)$ when $C = 1$. Energy is not good to verify the correctness of these two methods because it is not sensitive. The energies between $V = -1$ and 0 of different $C$ are same within error bar. We compare a more sensitive physical quantity, that is, the correlation function as shown in Table I. Here we choose $V = -0.5$ and $L = 32$. CF(r) means the correlation function (CF) along x axis, the distance is $r$. This also proves our
Another order parameters

There was another order parameter $P_+$ to distinguish the mixed and columnar states as shown in Ref.[18]. In dimer language, $S_+(q) \sim \sum_{j,k} e^{i q(r_j-r_k)} |\mathbb{I}_j \mathbb{I}_k \mathbb{I}_j \mathbb{I}_k|$. We have $P_+ = S_+({\pi, \pi})^{1/2}$ to characterize the plaquette or mixed state in general. At $V = -0.5$, we have a finite value even when $1/L \to 0$, as shown in Fig. 7. This result also prove the existence of mixed phase.

| $r$ | $C = -V$          | $C = 1$          |
|-----|------------------|------------------|
| 0   | 1.000000(000)    | 1.000000(000)    |
| 1   | -0.333333(000)   | -0.333333(000)   |
| 2   | 0.380892(136)    | 0.380276(340)    |
| 3   | -0.271613(040)   | -0.271686(120)   |
| 4   | 0.325661(231)    | 0.324952(569)    |
| 5   | -0.254040(074)   | -0.254015(202)   |
| 6   | 0.312379(291)    | 0.311470(676)    |
| 7   | -0.247721(103)   | -0.247862(273)   |
| 8   | 0.307659(336)    | 0.306816(755)    |
| 9   | -0.244968(132)   | -0.245125(314)   |
| 10  | 0.305604(361)    | 0.304557(803)    |
| 11  | -0.243631(158)   | -0.243511(346)   |
| 12  | 0.304598(379)    | 0.303333(784)    |
| 13  | -0.242977(179)   | -0.242679(326)   |
| 14  | 0.304154(390)    | 0.302762(822)    |
| 15  | -0.242729(188)   | -0.242411(335)   |
| 16  | 0.302465(998)    | 0.29796(295)     |

TABLE I. The correlation function $\text{CF}(r)$ along $x$ axis of square lattice QDM under two different choices about $C$, $T = 0.01$ $V = -0.5$ and $L = 32$.

FIG. 7. As size $1/L \to 0$, $P_+$ tends to a finite value at $V = -0.5$.

choice of $C$ when $V < -1$ is proper. In fact, the energies of these two methods are always similar on square lattice because ground states can be converted by pair update. However, on triangular lattice and other complex lattice, the energies will be significantly different due to the lack of ergodicity for the pair update ($C = -V$).

The original data of Fig. 4(a)

We have shown all the original data of Fig. 4(a) in Fig. 6(a) and (b). All parameters are the same as defined in Fig. 3(a).