Improved Sweeping Cluster Algorithm for Quantum Dimer Model

Zheng Yan\textsuperscript{1,2} \thanks{zhengyan@hku.hk}

\textsuperscript{1} Department of Physics and HKU-UCAS Joint Institute of Theoretical and Computational Physics, The University of Hong Kong, Pokfulam Road, Hong Kong
\textsuperscript{2} State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai 200438, China

Quantum dimer models (QDMs) featured by strong geometric constraint are effective low energy descriptions of many quantum spin systems. The geometric restriction described by local gauge field, hinders the application of numerical algorithms. Before sweeping cluster method was applied in world-line quantum Monte Carlo (QMC) algorithm, there is only projector QMC which obey the constraints and could be used for calculation on QDMs. However, the projector QMC for QDMs has some drawbacks, e.g., it is not effective when the parameter interval away from Rokhsar-Kivelson (RK) point. That’s because the projector method still lacks a cluster update to improve its efficiency. Although sweeping cluster algorithm improves the update for these systems, it also only works in one winding (topological) sector. In this paper, we improve the sweeping cluster method to sample in different winding sectors.

I. INTRODUCTION

A common theme in modern many-body physics is constraint which always arises when there is a particularly large energy scale in the Hamiltonian. We usually use gauge field theory to describe them in mathematics. However, the numerical calculation of the constrained models is difficult which directly delays our research and understanding for these many-body systems. Quantum dimer models (QDMs) featured by strong geometric restrictions are effective low energy descriptions of many quantum spin systems\cite{1–6}. The QDM Hamiltonian on square lattice can be written as

$$H = -\sum_{\text{plaq}} (\langle \mathbf{1} \rangle \langle \mathbf{1} \rangle + \text{H.c.}) + V \sum_{\text{plaq}} (\langle \mathbf{1} \rangle \langle \mathbf{1} \rangle + \langle \mathbf{z} \rangle \langle \mathbf{z} \rangle) \quad (1)$$

where the summations are taken over all elementary plaquettes of the lattice. This seemingly simple Hamiltonian contains strong geometric constraint which requires every site on the lattice to be covered by one and only one dimer. The QDM Hamiltonian on triangular and other lattices are similar to this, all satisfy this constraint, and are composed of kinetic energy (resonance between the dimers of a plaquette) and their potential energy.

Usually, there is a U(1)/Z2 gauge field on bipartite/nonbipartite QDM due to the restrictions. Take square/triangular lattice as examples, we can define winding number and winding sector for them as Fig.1\cite{6,9}. The different winding numbers describe different winding sectors on bipartite lattice. And the parity of the winding numbers determines the different winding sectors on nonbipartite lattice. It is obvious that local operator such as the Hamiltonian operator can not change the winding sector, only a global loop which cross through the boundary do as shown in Fig.2.

We developed an efficient and exact quantum Monte Carlo (QMC) based on stochastic series expansion (SSE) method \cite{10,12}. ”sweeping cluster” algorithm (SCA) \cite{13}, which automatically satisfies the constraint. Before sweeping cluster method was applied in world-line Monte Carlo (MC) algorithm, there is only projector MC which obey the constraints and could be used for calculation on QDMs \cite{14,16}. However, the projector MC for QDMs has some drawbacks, e.g., it is not effective when the parameter interval away from Rokhsar-Kivelson (RK) point. In fact, the projector method still lacks a cluster update to improve its efficiency. Comparing with projector MC, SCA solved the cluster update problem for constrained systems. However, it still only works in one winding sector which need to be improved. In many frustrated magnet cases, it is important to change the topological sectors, such as the phase diagram study of triangular lattices \cite{17}, Cantor deconfinement \cite{18} and the finite temperature study of QDM \cite{19}.

In this paper, we further develop the sweeping cluster algorithm to enable sampling between different winding sectors. In principle, this method works on any lattice QDM and can be generalized to other constrained models. In the following, we use the QDM on square lattice as examples to elaborate the details of this algorithm and provide simulations of square/triangular lattice QDM as
II. A SIMPLE INTRODUCTION OF SWEEPING CLUSTER UPDATE

Let’s briefly review sweeping cluster algorithm (SCA) base on SSE framework. The key idea of SCA is sweeping the configurations one by one along imaginary time and connecting two close configurations with update-lines and operator in the rule of MC, to keep the constraint as Fig. 2(I) shown.

![Diagram of sweeping cluster update](image)

FIG. 2. Left: A global loop update crosses through the boundary to change the winding number. Right: A local loop can not change the windling number.

We write the 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:

$$H_{1,p} = -V \left( |11\rangle\langle11| + |\bar{z}\rangle\langle\bar{z}| \right) + V + C,$$

$$H_{2,p} = \left( |00\rangle\langle00| + |\bar{z}\rangle\langle\bar{z}| |11\rangle\langle11| \right).$$

Here we have subtracted a constant $N_p(V+C)$ from Eq. (1). The constant $V+C$ should make all matrix elements of $H_{1,p}$ positive which means $C > \max(-V,0)$. We will choose $C = 1$ in this article for convenience.

The powers of $H$ in the SSE of the partition function $Z$ can be expressed as sums of products of the plaquette operators $H$ and $H$. Such a product is conveniently referred to by an operator-index sequence: $S_n = [a_1, p_1], [a_2, p_2], \ldots, [a_n, p_n]$, where $a_i \in \{1,2\}$ corresponds to the type of operator (1=diagonal, 2=off-diagonal) and $p_i \in \{1, \ldots, N_p\}$ is the plaquette index. It is also convenient to work with a fixed-length operator-index list with $M$ entries and to include the identity operator $[0,0]$ as one of the operator types.

The expanded partition function takes then the same form as the SSE in the spin models:

$$Z = \sum_{\alpha} \sum_{S_M} \beta^n (M-n)! \frac{1}{M!} \langle \alpha | \prod_{i=1}^{M} H_{a_i, p_i} | \alpha \rangle,$$

where $n$ is the number of operators $[a_i, p_i] \neq [0,0]$. Inserting complete sets of states between all the plaquette operators, the product can be written as a product of the following non-zero plaquette matrix elements:

$$\langle 11| H_{1,p} |11\rangle = \langle \bar{z} | H_{1,p} | \bar{z}\rangle = 1,$$

$$\langle 11| H_{2,p} | \bar{z}\rangle = \langle \bar{z} | H_{2,p} | 11\rangle = 1,$$

$$\langle \text{other} | H_{1,p} | \text{other}\rangle = 1 + V,$$

the $|\text{other}\rangle$ here means that plaquette $p$ has 1 or 0 dimer. Such matrix elements are depicted in Fig. 2II where the plaquette below(above) is the ket(bra).

Diagonal update is also similar as in spin models: We accept the insertion/deletion according to the Metropolis acceptance probabilities,

$$P_{\text{ins}} = \frac{N_p \beta^n |\alpha \rangle H_{1,p} |\alpha \rangle}{M-n},$$

$$P_{\text{del}} = \frac{M-n+1}{N_p \beta^n |\alpha \rangle H_{1,p} |\alpha \rangle}.$$
Choose a flippable plaquettes (FPs) randomly no matter it is diagonal or off-diagonal as starting operator vertex firstly. FP means the plaquette has two parallel dimers. Secondly, create four update-lines from every link of the plaquette, and all the lines go along one imaginary-time direction until they touch next vertex. The update-lines grow up in the imaginary-time direction will change the vertex configuration: The links touched by update-lines will create/cancel dimers as sweeping along imaginary-time. Thus the four initial update-lines rotate the two dimers of the original FP as they go along. The update-lines are extended until one or more of the update-lines hit another operator vertex from below.

Then, after updating the plaquette beneath on the new operator vertex according to the update-lines, we need to decide how to create or destroy update-lines to update the plaquette above and continue sweeping.

For this, there are three different processes to consider: (1) The new plaquette beneath is an FP, and the old plaquette above is not an FP. We can then change the plaquette above into an FP in two ways: either the resulting vertex will become diagonal or off-diagonal. We choose between these two possibilities shown in (c) and (d) in Fig. 3(II) with probability 1/2. (2) The new plaquette beneath is not an FP. Then change the upper plaquette to be same as the one underneath, as shown in (a), (b), (e) and (f) in Fig. 3(II). (3) Both the new plaquette beneath and the old plaquette above are FPs. Then there are two choices: the cluster-update ends if the number of total lines is four. If not, the four update-lines continue through the vertex and sweep on.

At the end of the sweeping cluster update, when the last four update-lines are deleted, we get a new configuration B with weight \( W_B \) to replace the old configuration A with weight \( W_A \). To ensure detailed balance, we must invoke a Metropolis accept/reject step \(^{20}\) on the whole cluster update with an acceptance probability. If we denote the number of operator vertices in configuration A with FPs on both sides by \( N_{\text{FP}} \), and the same amount in configuration B by \( N_{\text{FP}} + \Delta \), then

\[
P_{\text{accept}}(A \rightarrow B) = \min\left(\frac{N_{\text{FP}}}{N_{\text{FP}} + \Delta} \left(\frac{2}{1 + V}\right)^\Delta, 1\right). \tag{8}
\]

That’s all about the original sweeping cluster method. Although it works better than projector QMC methods before, it cannot change the winding sector while sampling. It means SCA still need to be improved.

**III. CONSTRUCT GLOBAL AND LARGE CLUSTER IN SWEEPING CLUSTER ALGORITHM**

Comparing with projector MC used before, SCA solved the cluster update problem for constrained systems. However, starting from a FP means all updates are derived from Hamilton’s dynamics which is local. In fact, the structure of QMC can be understood as imaginary time evolution of the classical dimer configuration, and SCA under QMC rules fully samples these evolution configurations. Based on the origin SCA, we can further generalize the directed loop algorithm of the N-dimensional classic dimer model to the N+1-dimensional QDM. We keep the same origin SCA method in diagonal update and cluster update. After diagonal update and cluster update, let us add a new step into the improved method.

At high temperature, there is an easy solution. After cluster update, walk randomly on the free links until a loop is formed and flip all links on it. The free links here means that there is no operator on it along imaginary time. It is worth noting that the loop here must be connected via one dimer and one empty link staggerly, and it may be local or global as Fig. 2. However, when temperature becomes low enough, there are less flippable free links and it becomes impossible to connect a loop. So we need to construct an effective global update method as Fig. 4 shown and its details is in flowing.

Firstly, choose a configuration at an certain imaginary time and do a directed loop as in classical dimer model\(^{21}\). We can start at a random chosen site and go through links with and without dimer one by one until it comes back to the start point and closed. In this step, you can repeat until getting a global loop if you wanna improve the effect of changing winding sectors. Then we get a random local/global loop in this configuration as shown in Fig. 2. Now all the links of this loop create update-lines instead of plaquette and begin to sweep the configurations along imaginary time direction. Here we should do it under a modified rules as following.

Secondly, all the update-lines meet the vertex should go on without stopping. There are also three different processes to consider which is same as original SCA: (1) The new plaquette beneath is an FP, and the old plaquette above is not an FP. We can then change the plaquette above into an FP in two ways: either the resulting vertex will become diagonal or off-diagonal. We choose between these two possibilities shown in (c) and (d) in Fig. 3(II) with probability 1/2. (2) The new plaquette beneath is not an FP. Then change the upper plaquette to be same as the one underneath, as shown in (a), (b), (e) and (f) in Fig. 3(II). (3) Both the new plaquette beneath and the old plaquette above are FPs. The four update-lines continue through the vertex and sweep on.

At last, if all the update-lines closed, head to tail meet, when the update-line come back to the start floor of imaginary time, the cluster is finished and accept it via the probability of Eq. (8). If the update-lines can not be closed, go on sweeping until they return to the start floor again. We can set a truncation number \( N \): When they return to the initial floor for the \( N \)-th time, give up the update if they are still not closed. At low temperature, \( N=1 \) is always enough and \( N \) can be set larger at higher \( T \).

Through the improved sweeping cluster in this step, we are equivalent to generalizing the classical directed loop algorithm to a high-dimensional space. On one hand, our
starting update element is no longer a flippable plaquette, but can be a loop of any size. On the other hand, if this loop walks along torus and is non-contractible, then we achieve sampling walks in spaces of different winding sectors. From the schematic diagram Fig.2, Hamiltonians evolve a loop layer by layer along imaginary time, and improved sweeping cluster method is to update this configuration as a whole.

In the case of finite temperature or on different sides of $V = 1$, sampling in different winding sectors is required as we known. The sector of ground state when $V < 1$ is $(0, 0)$, i.e. columnar case, and it becomes $(L/2, 0)$ or $(0, L/2)$, that is staggered case, during $V > 1$. It’s known that the energy of staggered phase should be zero which can be a strong criterion. As Fig.5 (a) shown, we see the ground state of ED and iSCA becomes from columnar sector to staggered sector in $V > 1$ while SCA stays in columnar sector. Both ED and iSCA work well near the topological first-order phase transition point ($V = 1$).

(b) At $V = 0.5$, the energy of iSCA which contains the information of all sectors matches well with the correct result of ED, but SCA is not right at finite temperature because the algorithm is confined in a sector.

People may think that the improving sweeping cluster algorithm is not efficient enough, because it requires all update-lines to be closed after whole imaginary time cycle due to the periodic boundary condition of imaginary time. Actually, this does a offer the effectiveness of the algorithm, especially when the size is larger. So a simpler way is that we can generalize it to the method of projector SSE Monte Carlo method[22, 23].

IV. IMPROVED SWEEPING CLUSTER ALGORITHM IN PROJECTOR SSE METHOD

The projector Monte Carlo algorithm[21] is a commonly numerical method for studying ground states of quantum many-body systems. In a broad sense, Green’s function Monte Carlo, diffusion Monte Carlo are both be-
long to it. Consider a state $|\Psi\rangle$ and its expansion in terms of eigenstates $|n\rangle$, $n = 0, 1, ..., $ of some Hamiltonian $H$;

$$|\Psi\rangle = \sum_n a_n |n\rangle$$  

(9)

Let $H$ be the Hamiltonian of interest. Then for sufficiently large $\beta$, $e^{-\beta H}$ can be used as a projection operator onto any state of this system.

$$\lim_{\beta \to \infty} e^{-\beta H} |\Psi\rangle = \lim_{\beta \to \infty} \sum_n e^{-\beta E_n} a_n |n\rangle = \lim_{\beta \to \infty} e^{-\beta E_0} \sum_n e^{-\beta(E_n-E_0)} a_n |n\rangle = \lim_{\beta \to \infty} e^{-\beta E_0} a_0 |0\rangle$$  

(10)

Then, from this expression, one can write a normalization of the ground state wavefunction like partition function, $Z = \langle 0|0 \rangle$ with two projected states (bra and ket) as,

$$Z = \lim_{\beta \to \infty} (\langle \Psi_L | e^{-\beta H} | \Psi_R \rangle) = \lim_{\beta \to \infty} \langle \Psi_L | e^{-2\beta H} | \Psi_R \rangle$$  

(11)

For convenience, in the following we use $\beta$ instead of $2\beta$. In order to represent the normalization as a sum of weights, $Z = \sum_n W(x)$, we use Handscomb’s power series expansion (PSE) and stochastic series expansion (SSE) framework to rewrite it as,

$$Z = \sum_{\Psi_L} \sum_{\Psi_R} \sum_{S_M} \frac{\beta^n (M-n)!}{M!} \left\langle \Psi_L \left| \prod_{i=1}^M H_{a_i, p_i} \right| \Psi_R \right\rangle ,$$  

(12)

$S_M = [a_1, p_1], [a_2, p_2], ..., [a_M, p_M]$, where $a_i \in \{1, 2\}$ corresponds to the type of operator ($1$ = diagonal, $2$ = off-diagonal) and $p_i \in \{1, ..., N_L\}$ is the index of position. It is convenient to work with a fixed-length operator-index list with $M$ entries and to include the identity operator $|0\rangle$ as one of the operator types. And $n$ is the number of operators $[a_i, p_i] \neq [0, 0]$. In this framework, we can apply the previous sweeping cluster method in SSE [13].

Then the steps are almost same with in finite temperature, the only difference is that the boundary condition of imaginary time becomes open. It means the global loop need not be same after $\beta$ evolution, i.e., the configuration and loop at $\tau = \beta$ need not be equal to ones at $\tau = 0$. However, the price is that it can only work at zero temperature.

On the triangular lattice QDM, we sweep the energy of several size under different parameter $V$ at zero temperature. When $V > 1$, the ground state is staggered phase without any parallel dimers in plaquette. This configuration cannot be obtained from the state of $V < 1$ through the evolution of local operators. And the energy of staggered state must be 0. So we can judge whether the transition of different topological is successful sectors via the energy near $V = 1$. It is worth noting that because the triangle lattice has more links on each lattice site, it is more difficult for either memory of ED or sampling of QMC.

As the Fig.6, the QMC simulation results of different sizes show that the sector of columnar phase can successfully enter the sector of staggered phase. It should be noted that under a certain size, the $\sqrt{12} \times \sqrt{12}$ phase will appear in the columnar sector, this article will not discuss and pay attention to this. In summary, improved SCA works better in the open boundary condition of imaginary time.

V. CONCLUSIONS

Numerical study of the quantum dimer model is important and notoriously difficult. We improve the sweeping cluster SSE method to calculate them. The technique keeps the geometric configuration satisfied by sweeping vertices in imaginary-time order and work in different winding sectors. In principle, this method works on any lattice QDM and can be generalized to other constrained models.

VI. ACKNOWLEDGEMENTS

I wish to thank Olav Syju˚ asen, Jie Lou, Yan Chen, Chenrong Liu, Ruizhen Huang, Zheng Zhou, Xue-Feng Zhang, Anders Sandvik and Zi Yang Meng for fruitful discussions. In addition, I also want to thank my parents who took care of my wife while she was pregnant, so that I can rest assured of scientific research. Acknowledge my wife’s gift, the birth of my son – YAN Gejie.
[1] D. S. Rokhsar and S. A. Kivelson, Phys. Rev. Lett. 61, 2376 (1988).
[2] G. Misguich, D. Serban, and V. Pasquier, Physical Review B 67, 214413 (2003).
[3] D. Poilblanc, M. Mambrini, and D. Schwandt, Physical Review B 81, 180402 (2010).
[4] Z. Yan, Z. Zhou, O. F. Syljuåsen, J. Zhang, T. Yuan, J. Lou, and Y. Chen, arXiv e-prints, arXiv:1911.05433 (2019), arXiv:1911.05433 [cond-mat.str-el].
[5] Z. Yan, Y.-C. Wang, N. Ma, Y. Qi, and Z. Y. Meng, arXiv preprint arXiv:2007.11161 (2020).
[6] R. Moessner and K. S. Raman, in Introduction to Frustrated Magnetism (Springer, 2011) pp. 437–479.
[7] X.-F. Zhang, S. Hu, A. Pelster, S. Eggert, et al., Physical review letters 117, 193201 (2016).
[8] Z. Zhou, D.-X. Liu, Z. Yan, Y. Chen, and X.-F. Zhang, arXiv preprint arXiv:2005.11133 (2020).
[9] Z. Zhou, C.-L. Liu, Z. Yan, Y. Chen, and X.-F. Zhang, arXiv preprint arXiv:2010.01750 (2020).
[10] A. W. Sandvik and J. Kurkijarvi, Physical Review B 43, 5950 (1991).
[11] A. W. Sandvik, Phys. Rev. B 59, R14157 (1999).
[12] O. F. Syljuåsen and A. W. Sandvik, Physical Review E 66, 046701 (2002).
[13] Z. Yan, Y. Wu, C. Liu, O. F. Syljuåsen, J. Lou, and Y. Chen, Phys. Rev. B 99, 165135 (2019).
[14] O. F. Syljuåsen, International Journal of Modern Physics B 19, 1973 (2005).
[15] O. F. Syljuåsen, Physical Review B 71, 020401 (2005).
[16] O. F. Syljuåsen, Physical Review B 73, 245105 (2006).
[17] A. Ralko, M. Ferrero, F. Becca, D. Ivanov, and F. Mila, Phys. Rev. B 71, 224109 (2005).
[18] E. Fradkin, D. A. Huse, R. Moessner, V. Oganesyan, and S. L. Sondhi, Physical Review B 69, 224415 (2004).
[19] F. S. Nogueira and Z. Nussinov, Physical Review B 80, 104413 (2009).
[20] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, The journal of chemical physics 21, 1087 (1953).
[21] F. Alet, J. L. Jacobsen, G. Misguich, V. Pasquier, F. Mila, and M. Troyer, Phys. Rev. Lett. 94, 235702 (2005).
[22] A. W. Sandvik, Physical review letters 95, 207203 (2005).
[23] A. W. Sandvik and H. G. Evertz, Physical Review B 82, 024407 (2010).
[24] R. Blankenbecler and R. Sugar, Physical Review D 27, 1304 (1983).
[25] D. Handscomb, in Mathematical Proceedings of the Cambridge Philosophical Society, Vol. 58 (Cambridge University Press, 1962) pp. 594–598.