Monte Carlo simulations of two-dimensional fermion systems with string-bond states

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We describe an application of variational Monte Carlo to two-dimensional fermionic systems within the recently developed tensor-network string-bond state (SBS) ansatz. We use a combination of variational Monte Carlo and stochastic optimization to optimize the matrix-product state matrices representing the ground state. We present results for a two-dimensional spinless fermion model including nearest-neighbor Coulomb interactions and determine using finite-size scaling the phase boundary between charge-ordered insulating and metallic phases. This approach can treat frustrated systems and be easily extended to for fermions with spin.

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I. INTRODUCTION

The properties of two dimensional (2D) and frustrated quantum many-body models play an important role in condensed matter physics. Numerical methods including quantum Monte Carlo (QMC)\textsuperscript{1,4} and the density matrix renormalization group (DMRG)\textsuperscript{2,4} have been essential in understanding the ground state and thermodynamic properties of interacting electron and spin systems. These two classes of methods have well known limitations however: QMC is severely limited to the systems that can be studied by the fermion sign problem, and DMRG methods are largely limited to one dimensional (1D) or quasi-1D systems.

Underlying DMRG methods is a matrix product state (MPS) representation of the quantum state. If each configuration in the wavefunction is written as \( |\Psi\rangle \) representation of the ground state. We present results for a two-dimensional spinless fermion model including nearest-neighbor Coulomb interactions and determine using finite-size scaling the phase boundary between charge-ordered insulating and metallic phases. This approach can treat frustrated systems and be easily extended to for fermions with spin.

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In Eq. \( \Psi \) the weight of each configuration is given by the trace of a product of \( D \times D \) matrices \( A^k_{jk} \). The advantage of using a MPS representation is that provides an accurate representation of the ground state of a 1D quantum system with only moderate values of \( D \). Eq. \( \Psi \) can be used to represent a 2D system by simply numbering the lattice sites in 2D sequentially (as in Fig. 1(a)), but favorable scaling with the matrix size \( D \) is then lost because the MPS ansatz can only describe entanglement along one chain direction.

A recent innovation is the use of Monte Carlo sampling to evaluate expectation values of the Hamiltonian as well as other operators within MPS-type trial states\textsuperscript{7–10}. By sampling the physical states of the system rather than contracting the matrices the computational scaling in \( D \) is reduced. Derivatives of the energy with respect to the matrix elements can also be calculated and then used to optimize the matrix elements \( A^k_{jk} \). The use of QMC sampling brings the computational advantage of trivial parallelization of Monte Carlo averages. While most applications have been to quantum spin models, this approach has successfully been used for more complicated quantum models such as the 1D Hubbard model where each site has four rather than two degrees of freedom\textsuperscript{11}.

Many variations of the MPS ansatz have been suggested to generalize it to 2D systems. The most natural extension to higher dimensions is to replace the matrices in Eq. \( \Psi \) by tensors and the trace by a more general contraction over the tensor indices. Projected entangled pair states (PEPS) are one such tensor network generalization\textsuperscript{12}. PEPS have been successfully applied to 2D frustrated spin models\textsuperscript{15,13}. A variation (iPEPS) has also been proposed for evaluating thermodynamic (infinite lattice) quantities\textsuperscript{14–18}. The main limitation in applying these methods is their poor computational scaling in the tensor size\textsuperscript{14,17}, typically \( \propto D^{12} \). An alternate approach is to use a somewhat more restricted ansatz that can be more easily computationally evaluated. The promise is that one can trade some complexity of the representation by increasing the number of variational parameters. Examples of this general approach include the multi-scale entanglement renormalization ansatz (MERA)\textsuperscript{18}, second renormalization of tensor networks\textsuperscript{19,20}, and tensor-renormalization group\textsuperscript{21,22} approaches.

In this paper we will explore a generalization of one such approach, the string-bond states (SBS) ansatz, where several one dimensional MPS “strings” of operators are placed in different directions on the 2D lattice\textsuperscript{23,24}. Applications to fermionic systems bring additional challenges to tensor network methods. In an occupation number representation the sign of each configuration necessarily depends on the ordering of the fermionic creation operators. While trivial in 1D where the Jordan-Wigner transformation can be used, the signs lead to long-range correlations between the tensors representing neighboring sites in 2D. One of the key questions is whether it is possible to come up with an effectively local tensor network scheme for fermions and to what degree the difficulty of doing this depends on the model in question.
The weight of a configuration in the SBS approximation is represented in terms of overlaps defined on a set of operator “strings” \{S\}:

\[
\langle C_n | \Psi \rangle = \prod_S \text{Tr} \left[ \prod_i S^i \right],
\]

where \( |C_n \rangle \) is a state in a local (e.g. occupation number) basis and \( S^i \) are \( D \times D \) matrices. As shown in Fig. 1 we use a set of two strings \{\(S_A, S_B\}\} to cover the lattice, each of which corresponds to the usual “snake” generalization conventionally used to adapt a MPS state to a 2D geometry. The string \(S_A\) (\(S_B\)) follows the hopping integrals aligned along \(x\) (\(y\)). The matrices for these two strings are labeled \(A\) and \(B\). The SBS representation for the wavefunction \(|\Psi\rangle\) is written as

\[
|\Psi\rangle = \sum_n W(C_n)|C_n\rangle,
\]

where \(W(C_n) = \prod_S W_S(C_n)\). The weights \(W_S(C_n)\) for the two strings are given by

\[
W_A(C_n) = \text{Tr} \prod_{i \in S_A} A^i = \text{Tr} \prod_{i_x=1}^{L} \left( \prod_{i_y=1}^{M} A^{M(i_x-1)+i_y} \right),
\]

\[
W_B(C_n) = \text{Tr} \prod_{i \in S_B} B^i = \text{Tr} \prod_{i_y=1}^{M} \left( \prod_{i_x=1}^{L} B^{M(i_y-1)+i_x} \right),
\]

where \(i_x\) and \(i_y\) correspond to the \(x\) and \(y\) coordinates of site \(i = (i_x, i_y)\) for a \(L \times M\) rectangular lattice with the total number of lattice sites \(N\).

The variational Monte Carlo (MC) method we use to evaluate the energy and other correlation functions is based on the method of reference 5. We have previously shown that this method can be generalized to 1D fermionic systems, where the weight of a configuration is given by a MPS, i.e. a single string. Configurations \(|C_n\rangle\) are sampled according to the weight \(W(C_n)^2\). MC updates consist of interchanges of electrons of a given spin between neighboring sites. Updates are attempted first along the path of string \(S_A\) and then along the direction of string \(S_B\). In this manner, a system of “left” and “right” matrices can be used to efficiently perform the MC sampling.

We create a series of left matrices \(L_A^{i_x,i_y} = A^i L_A^{i_x,i_y+1}\) and \(L_B^{i_x,i_y} = B^i L_B^{i_x,i_y+1}\) for \(i_x = 1, \ldots L\) and \(i_y = 1, \ldots M\). Sequentially visiting the site \(i = (i_x, i_y)\) in either horizontal \(x\) (for \(S_A\)) or vertical \(y\) (for \(S_B\)) direction, we attempt to interchange electrons between that site and its nearest neighbor \(j = (j_x, j_y)\) until we have arrived at site \(N = (L, M)\). If a update is accepted (or rejected) according an acceptance probability \(p(C_n \to C_{n'}) = \min[W^2(C_{n'})/W^2(C_n),1]\), the right matrices \(R_A^{i_x,i_y} = R_A^{i_x,i_y-1} A^i\) and \(R_B^{i_x,i_y} = R_B^{i_x,i_y-1} B^i\) are advanced, respectively. Once the \(R\) matrices for a given string have been stored, measurements of the energy and derivatives of the energy are are implemented by traversing the string in the reverse direction.

II. METHOD

For a generic Hubbard-type model we decompose the Hamiltonian into two terms,

\[
H = H_0 + H_1,
\]

where diagonal \(H_0\) and off-diagonal \(H_1\) terms are given by

\[
H_0 = \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{\langle i,j \rangle} V_{ij} n_{i\uparrow} n_{j\downarrow},
\]

\[
H_1 = - \sum_{\langle i,j \rangle} t_{ij} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right).
\]

In Eq. 3 \(c_{i\sigma}^\dagger\) (\(c_{i\sigma}\)) create (annihilate) an electron of spin \(\sigma\) on site \(i\), \(n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}\), and \(n_i = n_{i\uparrow} + n_{i\downarrow}\). We assume here that the nearest neighbor sites in \(H_1\) are those on a conventional square lattice, although as discussed later, it is possible to generalize this to other periodic lattices. \(U\) and \(V_{ij}\) are on-site and intersite Coulomb interactions.
The energy estimator for the configuration $C_n$ is

$$E(C_n) = \sum_{C_{n'}} W(C_{n'}) W(C_n) \langle C_{n'} | H | C_n \rangle. \tag{8}$$

In Eq. (8) the diagonal part of the energy $\langle H_0 \rangle$ can simply be measured as an average over the configurations visited. Interchanges of electrons give contributions to the off-diagonal terms $\langle H_1 \rangle$. In calculating the matrix element in Eq. (8) a sign due to fermion exchange must be included.

Within the MPS representation the derivative of the energy with respect to the each of the matrix elements can easily be calculated. For the $A$ matrices of $S_A$ this derivative is

$$\frac{\partial E}{\partial A_{ij}^k} = 2 \left( \frac{E(C_n) - \langle E(C_n) \rangle}{W_A(C_n)} \frac{\partial W_A(C_n)}{\partial A_{ij}^k} \right), \tag{9}$$

where the derivatives of each trace can be written as

$$\frac{\partial W_A(C_n)}{\partial A_{ij}^k} = \frac{1}{1 + \delta_{ij}} \left[ Q^A_{ij}(k) + Q^A_{ji}(k) \right], \tag{10}$$

using $Q^A(k) = \prod_{i \neq k} A_i^k$. An identical expression is used for derivatives of the energy with respect to the $B$ matrices.

The matrix elements $A_{ij}^k$ and $B_{ij}^k$ for $k = 1, \ldots, N$ are first initialized to random numbers in the interval $[-\frac{1}{2}, \frac{1}{2}]$. We normalize the matrices so that their Frobenius norm is unity, i.e. $\frac{1}{2} \text{Tr}(AA^T) = 1$. MC measurements for the energy, derivatives, and other correlation functions are block-averaged as usual. After each block, matrix elements are updated using a stochastic optimization scheme. Each matrix element $A_{ij}^k$ is modified by a random amount in the direction indicated by the derivative of the energy,

$$A_{ij}^k \to A_{ij}^k - \delta \cdot R \cdot \text{sgn} \left( \frac{\partial E}{\partial A_{ij}^k} \right) \theta \left( \left| \frac{\partial E}{\partial A_{ij}^k} \right| - \alpha \right). \tag{11}$$

Here $R$ is a random number in the interval $[0, 1]$, $\text{sgn}(x)$ is the signum function of a real number $x$, and $\theta(x)$ is the unit step function. The parameter $\alpha$ restricts changes to only the matrix elements that have the most significant effect on the energy, those with the largest magnitude derivatives. We found that a small reduction in energy with a suitable choice of $\alpha$ is the most significant effect on the energy. Those with the largest magnitude derivatives. We found that a small reduction in energy with a suitable choice of $\alpha$ was obtained. Several MC blocks each followed by the update in Eq. (11) are then combined into one step labeled by the index $k$ of the optimization algorithm (see Fig. 2). At each successive $k$ the parameters $\delta$ and $\alpha$ are decreased by a multiplicative factor $Q$. For the results here, we typically used $Q = 0.9$. $\delta$ and $\alpha$ were initially chosen as 0.5. Simultaneously the number of MC blocks per step, $G(k)$, and samples per block, $F(k)$, are increased linearly. We typically used $F(k) = 5000-10000$ and $G(k) = 250-500$. This procedure gives an “annealing” procedure that for a sufficiently large $k$ should approach the global minimum energy. The MC sampling was parallelized using an “embarrassingly parallel” algorithm. The results presented here used up to 192 processors.

### III. RESULTS

We consider spinless fermions on a 2D square lattice interacting with a nearest-neighbor Coulomb repulsion. The Hamiltonian is given by

$$H = -t \sum_{\langle ij \rangle} (c_i^+ c_j + H.c.) + V \sum_{ij} n_i n_j. \tag{12}$$

In Eq. (12) $c_i^+$ creates a fermion on site $i$; sites $i$ and $j$ in $\langle ij \rangle$ are nearest-neighbor pairs on a 2D square lattice of $N$ sites with periodic boundary conditions. All energies will be given in units of $t$. We consider the half-filled case with $N/2$ particles. For this density, the $V$ interaction causes a checkerboard pattern charge-ordered (CO) insulating phase. In the 1D limit the model may be transformed via the Jordan-Wigner transformation to a spin-$\frac{1}{2}$ XXZ Heisenberg model and it can be shown exactly that the CO phase occurs when $V > V_c$ with $V_c = 2$. In 2D
where a single MPS can be used to represent the wave-matrix elements. In comparison with quasi-1D systems calculation, each starting with different random initialization calculations for systems up to 32 sites. Fig. 2(a) shows the relative error in the ground state energy, $\Delta E$ shows the relative error in the ground state energy, $\Delta E = |E_{\text{QMC}} - E_{\text{exact}}| / E_{\text{exact}}$, as a function of algorithm steps $k$ and matrix size $D$ for a $4 \times 4$ lattice. The interaction strength $V = 0.45$ chosen here is close to the CO transition point representing the most computationally challenging parameter region of the model. Here and in our following results, each value of $D$ is a separate calculation, each starting with different random initial matrix elements. In comparison with quasi-1D systems where a single MPS can be used to represent the wave-

$$V_c$$ is not known exactly. Analytical work using a slave-boson approximation was done for a model with SU(N) fermions. For the case of a 2D square lattice and taking $N = 2$ (corresponding to spin-$\frac{1}{2}$) the corresponding $V_c = 0.69$. This model was also previously studied using finite-temperature determinantal QMC down to temperatures of order $T \approx 0.5$. These numerical results were also compared with the mean-field RPA predictions, if one extrapolates the strong-coupling RPA result from reference 31 to $T = 0$, $V_c \approx 1/\sqrt{3} \approx 0.58$. The finite-temperature QMC results for $V_c$ appear to be consistent with this limit if an almost-linear extrapolation in the $T - V$ plane is assumed, but could not rule out the possibility that $V_c \to 0$ as $T \to 0$. As shown below, our present results are consistent with a nonzero $V_c$.

We compared the SBS-QMC results to exact diagonalization calculations for systems up to 32 sites. Fig. 2(a) shows the relative error in the ground state energy, $\Delta E = |E_{\text{QMC}} - E_{\text{exact}}| / E_{\text{exact}}|$, as a function of algorithm steps $k$ and matrix size $D$ for a $4 \times 4$ lattice. The interaction strength $V = 0.45$ chosen here is close to the CO transition point representing the most computationally challenging parameter region of the model. Here and in our following results, each value of $D$ is a separate calculation, each starting with different random initial matrix elements. In comparison with quasi-1D systems where a single MPS can be used to represent the wave-

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function (see Fig. A-1 of Reference 11), we found nearly comparable scaling of accuracy with respect to $D$ for the 2D system considered here.

An order parameter for the CO phase is the charge structure factor $S(q)$ for $q = (\pi, \pi)$, where $S(q)$ is defined as

$$S(q) = \frac{1}{N} \sum_{j,k} \langle n_j - \frac{1}{2} \rangle \langle n_k - \frac{1}{2} \rangle.$$ (13)

Fig. 2(b) shows the relative error in $S$, $\Delta S = |S_{\text{QMC}} - S_{\text{exact}}| / S_{\text{exact}}$, for a $4 \times 4$ lattice at the ordering wavevector $q = (\pi, \pi)$.

Fig. 3(a) and (b) further show the relative errors as a function of matrix size $D$ for larger system sizes that can still be solved exactly. As expected and seen in Fig. 3 for larger systems larger values of $D$ are required to reach the same accuracy. In all of the comparisons in Figs. 2 and 3 of order 100 algorithm steps were needed to converge the energy to within a relative energy accuracy of order $10^{-4}$. We also verified that restarting the optimization from the converged matrices gave no further improvement in the energy. Fig. 4 shows the convergence with $D$ for the largest system studied, $12 \times 12$, with $V = 0.8$. As shown in the inset, $S(\pi, \pi)$ scales as approximately $1/D^2$.

In the CO phase $S(\pi, \pi)/N$ converges to a finite value in the thermodynamic limit. Fig. 4 shows the finite-size scaling of $S(\pi, \pi)/N$. The results in Fig. 4 used up to $D = 64$ matrices and clearly show that a finite critical coupling $V_c$ for the CO phase exists. By plotting the extrapolated $S(\pi, \pi)/N$ versus $V$, we estimate that $V_c$ for the CO transition is $V_c = 0.45 \pm 0.02$

IV. DISCUSSION

In this paper we have presented numerical results using the SBS ansatz applied to a 2D fermionic model. In order to simulate a fermionic system, we have not attempted to make the sign pattern local, but instead have
simply used stochastic optimization to optimize both the sign and amplitude of a general SBS wavefunction. Because the computational scaling of the method is relatively small (proportional to $ND^4$), this “brute force” optimization is successful for reasonably large fermionic systems, for example here up to $N=144$. As the method is not restricted to unfrustrated lattices, we expect it will provide a useful way to study frustrated Hubbard-type models on lattice sizes out of reach of exact diagonalization. In comparison with DMRG which is more accurate on rectangular lattices of large aspect ratio, the SBS-QMC method can be used on square periodic lattices which are the easiest to perform finite-size scaling on.

While we have presented data here for a spinless fermion model, we are presently testing the method for 2D frustrated models including spin. Incorporating spin simply increases the number of states per site, which we find requires a somewhat larger $D$ to obtain comparable accuracy in the energy and correlation functions. Further improvements on the algorithm also can certainly be made. In applying SBS to 2D spin systems, it was noticed that the initial choice for the matrix elements could make a large difference in the convergence. Here we have only used random starting matrices—using a mean-field solution as the initial starting state could potentially improve the results.

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