Improving the Gutzwiller Ansatz with Matrix Product States

Sebastiano Peotta and Massimiliano Di Ventra

1 Department of Physics, University of California-San Diego, La Jolla, CA 92093, USA

The Gutzwiller variational wavefunction (GVW) is commonly employed to capture correlation effects in condensed matter systems such as ferromagnets, ultracold bosonic gases, correlated superconductors, etc. By noticing that the grand-canonical and number-conserving Gutzwiller Ansätze are in fact the zero-order approximation of an expansion in the truncation parameter \( \epsilon \) of a Matrix Product State (MPS), we argue that MPSs, and the algorithms used to operate on them, are not only flexible computational tools but also a unifying theoretical framework that can be used to generalize and improve on the GVW. In fact, we show that a number-conserving GVW is less efficient in capturing the ground state of a quantum system than a more general MPS which can be optimized with comparable computational resources. Moreover, we suggest a corrected time-dependent density matrix renormalization group algorithm that ensures the conservation of the expectation value of the number of particles when a GVW or a MPS are not explicitly number-conserving. The GVW dynamics obtained with our algorithm compares very well with the exact one in 1D. Most importantly, the algorithm works in any dimension for a GVW. We thus expect it to be of great value in the study of the dynamics of correlated quantum systems.

I. INTRODUCTION

The Gutzwiller variational wavefunction (GVW) has been an important tool in the analysis of various correlated quantum systems, ranging from ferromagnets to ultracold bosonic gases, to superconductors, etc. By noticing that the grand-canonical and number-conserving Gutzwiller Ansätze are in fact the zero-order approximation of an expansion in the truncation parameter \( \epsilon \) of a Matrix Product State (MPS), we argue that MPSs, and the algorithms used to operate on them, are not only flexible computational tools but also a unifying theoretical framework that can be used to generalize and improve on the GVW. In fact, we show that a number-conserving GVW is less efficient in capturing the ground state of a quantum system than a more general MPS which can be optimized with comparable computational resources. Moreover, we suggest a corrected time-dependent density matrix renormalization group algorithm that ensures the conservation of the expectation value of the number of particles when a GVW or a MPS are not explicitly number-conserving. Here, we extend the GVW to any dimension for general MPSs that do not explicitly conserve the particle number or other conserved quantities corresponding to Abelian symmetries of the Hamiltonian. Our algorithm can find applications in the study of correlated effects in quantum systems in dimension one and higher, both as a simple starting point and as a yardstick for more refined calculations. Indeed, the GVW is a variational mean-field wavefunction, and it is expected to work even better with increasing dimension.

I. INTRODUCTION

The Gutzwiller variational wavefunction (GVW) has been an important tool in the analysis of various correlated quantum systems, ranging from ferromagnets to ultracold bosonic gases, to superconductors, etc. By noticing that the grand-canonical and number-conserving Gutzwiller Ansätze are in fact the zero-order approximation of an expansion in the truncation parameter \( \epsilon \) of a Matrix Product State (MPS), we argue that MPSs, and the algorithms used to operate on them, are not only flexible computational tools but also a unifying theoretical framework that can be used to generalize and improve on the GVW. In fact, we show that a number-conserving GVW is less efficient in capturing the ground state of a quantum system than a more general MPS which can be optimized with comparable computational resources. Moreover, we suggest a corrected time-dependent density matrix renormalization group algorithm that ensures the conservation of the expectation value of the number of particles when a GVW or a MPS are not explicitly number-conserving. Here, we extend the GVW to any dimension for general MPSs that do not explicitly conserve the particle number or other conserved quantities corresponding to Abelian symmetries of the Hamiltonian. Our algorithm can find applications in the study of correlated effects in quantum systems in dimension one and higher, both as a simple starting point and as a yardstick for more refined calculations. Indeed, the GVW is a variational mean-field wavefunction, and it is expected to work even better with increasing dimension.

I. INTRODUCTION

The Gutzwiller variational wavefunction (GVW) has been an important tool in the analysis of various correlated quantum systems, ranging from ferromagnets to ultracold bosonic gases, to superconductors, etc. By noticing that the grand-canonical and number-conserving Gutzwiller Ansätze are in fact the zero-order approximation of an expansion in the truncation parameter \( \epsilon \) of a Matrix Product State (MPS), we argue that MPSs, and the algorithms used to operate on them, are not only flexible computational tools but also a unifying theoretical framework that can be used to generalize and improve on the GVW. In fact, we show that a number-conserving GVW is less efficient in capturing the ground state of a quantum system than a more general MPS which can be optimized with comparable computational resources. Moreover, we suggest a corrected time-dependent density matrix renormalization group algorithm that ensures the conservation of the expectation value of the number of particles when a GVW or a MPS are not explicitly number-conserving. Here, we extend the GVW to any dimension for general MPSs that do not explicitly conserve the particle number or other conserved quantities corresponding to Abelian symmetries of the Hamiltonian. Our algorithm can find applications in the study of correlated effects in quantum systems in dimension one and higher, both as a simple starting point and as a yardstick for more refined calculations. Indeed, the GVW is a variational mean-field wavefunction, and it is expected to work even better with increasing dimension.
the algorithm only for the GVW since the corresponding more general version for MPSs is simply notationally more involved. Finally, we conclude in Sec. V.

II. MATRIX PRODUCT STATES

Although not limited to this case, in the following we consider a quantum system defined on a open lattice of length $L$ where the lattice site $i$ can be occupied by a number $n_i = 0, \ldots, +\infty$ of bosons. The Hamiltonian is assumed to be the sum of nearest-neighbor terms which globally conserve the total number of particles $N = \sum n_i$. A typical example is the Bose-Hubbard Model:

$$
\hat{H}_{\text{BHM}} = -J \sum_i \left( \hat{b}_i^\dagger \hat{b}_{i+1} + \hat{b}_{i+1}^\dagger \hat{b}_i \right) + U \sum_i n_i, 
$$

(1)

containing a local interaction – being a function of the number operator $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ – that conserves the total number of particles. In the hopping term $\hat{b}_i^\dagger \hat{b}_{i+1}$ the operator $\hat{b}_i^\dagger$ destroys a particle on site $i + 1$ and the operator $\hat{b}_i^\dagger$ creates one particle on site $i$, again conserving $N$.

Before proceeding, let us first introduce some notations for the benefit of the reader. In the following a bold symbol $\mathbf{B}^{(i)}$ is a short hand for a tensor (or matrix) attached to site $i$ with two link indices, denoted by $\ell_{i-1}, \ell_i$ and components $B_{\ell_{i-1}, \ell_i}$. The link index $\ell_i$ is relative to the link connecting site $i$ and site $i + 1$ while $\ell_{i-1}$ refers to the link between site $i - 1$ and site $i$. Every link index $\ell_i$ ranges from 1 up to the link dimension $m_i$, thus the matrix $\mathbf{B}^{(i)}$ has dimension $m_i \times m_i$. $\mathbf{A}^{[n]}$ is a collection of tensors, one for each value of the occupation number $n_i$ attached to site $i$. For an inhomogeneous system $\mathbf{A}^{[n_1]} \neq \mathbf{A}^{[n_2]}$ in general, if $i \neq j$. The dot “.” has the meaning of a contraction of a link index $\ell_i$

$$
\left[ \mathbf{A}^{[n_1]} \cdot \mathbf{A}^{[n_2]} \right]_{\ell_{i-1} \ell_{i+1}} = \sum_{\ell_{i-1}, \ell_i} \mathbf{A}^{[n_1]}_{\ell_{i-1}, \ell_i} \mathbf{A}^{[n_2]}_{\ell_i, \ell_{i+1}}. 
$$

(2)

A set $\{ \mathbf{A}^{[n_i]} \}_{i=1, \ldots, L}$ is called a Matrix Product State (MPS), an alternative way to specify a wavefunction $|\Psi\rangle$. For an arbitrary given set of occupancies $\{ n_i \}_{i=1, \ldots, L}$ the complex number $\langle \{ n_i \} |\Psi\rangle$ is obtained by contracting all the link indices

$$
\langle n_1, n_2, \ldots, n_{L-1}, n_L |\Psi\rangle = \mathbf{A}^{[n_1]} \cdot \mathbf{A}^{[n_2]} \cdots \mathbf{A}^{[n_{L-1}]} \cdot \mathbf{A}^{[n_L]}.
$$

(3)

For open boundary conditions the leftmost link index $\ell_0$ and the rightmost one $\ell_L$ have dimensions $m_0 = m_L = 1$ and do not need to be contracted. Note that the exact ground state wavefunction has always an exact MPS representation but with impractically large values of $m_i$ for long chains ($L \gtrsim 20$). Therefore, reducing the link dimension $m_i$ with some sort of truncation procedure is the essential idea of MPS-based algorithms like DMRG.

It is computationally more convenient to restrict the Hilbert space only to the subspace of states with a fixed number of particles $N (\langle \{ n_i \} |\Psi\rangle = 0 \text{ for } \sum n_i \neq N)$. By explicitly enforcing this condition on the MPS (3) results in a block structure for the matrices $\mathbf{A}^{[n_i]}$ described in the following. The $i$-th link is divided in symmetry multiplets labeled by an integer $\alpha_i$, which is the number of particles located on sites at the left of the $i$-th link. Each multiplet has a multiplicity $d_{\alpha_i}$, which can be zero, and the values of the link index $\ell_i$ can be grouped accordingly, namely $\ell_i = (\alpha_i, k_{\alpha_i})$ with $1 \leq k_{\alpha_i} \leq d_{\alpha_i}$ and $\sum_{\alpha_i} d_{\alpha_i} = m_i$.

We denote by $\mathbf{A}^{[n_i]}_{\alpha_i-\alpha_i}$ the submatrix of $\mathbf{A}^{[n_i]}$ corresponding to the multiplets $\alpha_{i-1}$ on the $(i-1)$-th link and $\alpha_i$ on the $i$-th link. The definition of $\alpha_i$ leads to the condition $\alpha_0 = n_i + \alpha_{i-1}$ for $\alpha_{i-1} \alpha_i$ to be nonzero, thus large blocks of $\mathbf{A}^{[n_i]}$ are zero and the size of the MPS is greatly reduced. At the left boundary only the sector $\alpha_0 = 0$ has nonzero multiplicity $d_{\alpha_0} = 1$ and the same holds for $\alpha_L = N$ at the right boundary. A MPS with a block structure induced by a $U(1)$ (abelian) symmetry is easier to optimize since the dimension of the local eigenvalue problem to be solved is drastically reduced. Moreover one can perform several singular value decomposition (SVD) on each block instead of a more time consuming single SVD on a large matrix, an operation routinely performed during an imaginary- or real-time evolution.

III. GUTZWILLER ANSATZ AS A MATRIX PRODUCT STATE

For a bosonic system a commonly employed approximation is the grand-canonical Gutzwiller variational wavefunction ($\mu$-GVW)

$$
|\Psi\rangle_{\mu-\text{GVW}} = \bigotimes_i |\Psi_i\rangle |\Psi_i\rangle = \sum_i c_i^{(i)} |n_i\rangle. 
$$

(4)

The state $|n_i\rangle$ is an eigenstate of the number operator $\hat{n}_i |n_i\rangle = n_i |n_i\rangle$ and the $c_i^{(i)}$ are arbitrary variational parameters.

We immediately note that the grand-canonical Gutzwiller Ansatz is the most general MPS with link dimension $m_i = 1$ for every link $i$, since the matrix $\mathbf{A}^{[n_i]} = c_i^{(i)}$ becomes a simple scalar. From a $\mu$-GVW one can easily derive a canonical (number conserving) Gutzwiller Ansatz which we call $(n$-GVW)

$$
|\Psi\rangle_{n-\text{GVW}} = \frac{\mathcal{P}_N |\Psi\rangle_{\mu-\text{GVW}}}{\| \mathcal{P}_N |\Psi\rangle_{\mu-\text{GVW}} \|} \sim \int_0^{2\pi} d\phi e^{-i N \phi} \bigotimes_i \left( e^{i \hat{n}_i \phi} |\Psi_i\rangle \right).
$$

(5)
The $n$-GVW shows pronounced density oscillations with constant amplitude throughout the chain. On the contrary the more general MPS Ansatz is able to capture the quantum fluctuations that lead to a suppression of the oscillations. Right: link dimension $m_i$ for the same variational wavefunctions used for the left panel. Note that the $n$–GVW has a link dimension comparable to that of a MPS with $\epsilon = 10^{-5}$, but the latter is more efficient in describing the ground state as it can be seen from the variational ground state energy shown in Fig. 2.

An important observation is that particle number conservation alone has the nontrivial effect of increasing the amount of entanglement of the trial wavefunction. For a $\mu$–GVW $m_i = 1$ for all links and the block entropy\cite{16} is identically zero. On the other hand for a $n$–GVW one has $m_i = \sum_{\alpha_i=1}^{N+1} d_{\alpha_i} \leq N + 1$. Thus the block entropy is bounded by $\log(N + 1)$ and nonzero in general, unless each particle is localized on a single site. This implies that a $n$–GVW is computationally more expensive than a $\mu$–GVW.

An interesting question is then if a more general MPS - where the degeneracies $d_{\alpha_i}$ of the symmetry multiplets are not bounded ($d_{\alpha_i} \leq 1$) - can better capture the ground-state wavefunction at a comparable computational cost, where the computational cost of a MPS is roughly quantified by the link dimension $m_i$. In the following, we will indeed show that the answer is affirmative.

To show this explicitly, we consider $N = 20$ particles in a lattice of $L = 200$ sites with Hamiltonian given by Eq. (1) with $U/J = 2.0$ and, by using the standard DMRG algorithm, we optimize the $n$–GVW. The results are compared with MPSs with fixed discarded weight\cite{16} $\epsilon$, meaning that after each SVD the discarded singular values satisfy

$$\sum_{\text{discarded}} \sigma_i^2 < \epsilon.$$ \hfill (7)

In Fig. 1 we show the density profiles $n_i$ and the link dimensions $m_i$ relative to a $n$–GVW and MPSs. Pronounced density oscillations with constant amplitude are visible in the profile obtained with an optimized $n$–GVW. These oscillations are in fact a charge density wave induced by the repulsive Hubbard interaction.
corrected

\[ \langle N \rangle(t) \approx e^{i \Delta t \hat{H}_{\text{odd}}/2} e^{i \Delta t \hat{N}_{\text{even}}} e^{i \Delta t \hat{H}_{\text{odd}}/2}, \]

and it is possible to separately apply

\[ \exp(i \Delta t \hat{N}_{\text{even}}) = \bigotimes_{i} \exp(i \Delta t \hat{n}_{2i, 2i+1}), \]

\[ \exp(i \Delta t \hat{N}_{\text{odd}}) = \bigotimes_{i} \exp(i \Delta t \hat{n}_{2i-1, 2i}), \]

by updating two MPS matrices at a time

\[ M^{[n_i', n_{i+1}']} = \sum_{n_i, n_{i+1}} [\exp(i \Delta t \hat{H}_{\text{odd(even)}})]^{n_i', n_{i+1}'} A^{[n_i]} \cdot A^{[n_{i+1}']}. \]

In order to keep the MPS dimensions bounded one finds the best rank \( m \) approximation \( B^{[n_i]} : B^{[n_{i+1}]} \) of \( M^{[n_i, n_{i+1}]} \) by minimizing the functional

\[ \| M^{[n_i, n_{i+1}]} - B^{[n_i]} \cdot B^{[n_{i+1}]} \|^2, \]

where \( B^{[n_i]} \) (\( B^{[n_{i+1}]} \) are matrices with dimension \( m_{i-1} \times m_i \) (\( m_i \times m_{i+1} \)). The optimal solution is then obtained by retaining the largest \( m_i \) singular values of \( M^{[n_i, n_{i+1}]} \) (for more details see Ref. 16). The expectation value of \( \hat{N} \) calculated with the new MPS \( A^{[n_i]} \cdot A^{[n_{i+1}]} \to M^{[n_i, n_{i+1}]} \) is unchanged since \( \exp(i \Delta t \hat{H}_{\text{odd(even)}}) \) is a number-conserving operator but this is not necessarily true for the low rank approximation \( A^{[n_i]} \cdot A^{[n_{i+1}]} \to B^{[n_i]} \cdot B^{[n_{i+1}]} \).

In the following we specialize to the case of a \( \mu \)-GFW which nothing prevents to extend the algorithm presented.
in the following to a MPS that does not explicitly conserves the number of particle. A working implementation of the algorithm for the GVW is provided in Ref. 31.

We propose to minimize the functional

\[
\left\| \mathcal{H} |\Psi_i\rangle |\Psi_{i+1}\rangle - |\Phi_i\rangle |\Phi_{i+1}\rangle \right\|^2 - \mu \langle \Phi_i | \hat{n}_i | \Phi_i \rangle + \langle \Phi_{i+1} | \hat{n}_{i+1} | \Phi_{i+1} \rangle \tag{13}
\]

with respect to |\Phi_i\rangle and |\Phi_{i+1}\rangle which are assumed to be normalized (the normalization condition can be enforced by additional Lagrange multipliers that will be introduced below). The operator \( \mathcal{U} = 1 + O(\Delta t) \) is a generic evolution operator acting on two sites and sufficiently close to the identity. The Lagrange multiplier \( \mu \) is introduced in order to enforce the condition of particle number conservation

\[
\langle \Phi_i | \hat{n}_i | \Phi_i \rangle + \langle \Phi_{i+1} | \hat{n}_{i+1} | \Phi_{i+1} \rangle = \langle \Psi_i | \hat{n}_i | \Psi_i \rangle + \langle \Psi_{i+1} | \hat{n}_{i+1} | \Psi_{i+1} \rangle. \tag{14}
\]

Varying the functional (13) with respect to |\Phi_i\rangle and |\Phi_{i+1}\rangle gives two coupled equations

\[
|\Phi_i\rangle = \frac{\varepsilon_1}{1 + \lambda \hat{n}_i} |\Phi_{i+1} \rangle \mathcal{U} |\Psi_i\rangle |\Psi_{i+1}\rangle, \tag{15}
\]

\[
|\Phi_{i+1}\rangle = \frac{\varepsilon_2}{1 + \lambda \hat{n}_{i+1}} |\Phi_i \rangle \mathcal{U} |\Psi_i\rangle |\Psi_{i+1}\rangle. \tag{16}
\]

The additional Lagrange multipliers \( \varepsilon_1 \) and \( \varepsilon_2 \) are used to preserve the normalization condition

\[
\langle \Phi_i | \Phi_i \rangle = \langle \Phi_{i+1} | \Phi_{i+1} \rangle = 1. \tag{17}
\]

The parameter \( \lambda \) is proportional to \( \mu \) and must be adjusted to ensure the validity of Eq. (14). The coupled equations (14), (15), (16) and (17) in the unknowns |\Phi_i\rangle, |\Phi_{i+1}\rangle, \lambda, \varepsilon_1, \varepsilon_2 \) can be solved iteratively. The first step in the iterative procedure is to first solve the equations for \( \lambda = 0 \). This is nothing else than the usual TDMRG algorithm where \( \tilde{U} |\Psi_i\rangle |\Psi_{i+1}\rangle \sim |\Phi_i^{(0)}\rangle |\Phi_{i+1}^{(0)}\rangle \) is approximated by truncating to the largest \( m_i \) singular values \( (m_i = 1 \) in the case of a \( \mu \)-GVW). The couple of states obtained in such a way are the first of a sequence |\Phi_i^{(j)}\rangle |\Phi_{i+1}^{(j)}\rangle \) constructed as follows.

Define the non-normalized states

\[
|\phi_i(\lambda)\rangle = \frac{1}{1 + \lambda \hat{n}_i} \langle \Phi_i^{(j)} \rangle \mathcal{U} |\Psi_i\rangle |\Psi_{i+1}\rangle, \tag{18}
\]

\[
|\phi_{i+1}(\lambda)\rangle = \frac{1}{1 + \lambda \hat{n}_{i+1}} \langle \Phi_i^{(j)} \rangle \mathcal{U} |\Psi_i\rangle |\Psi_{i+1}\rangle. \tag{19}
\]

and find the solution \( \lambda^* \) of the equation

\[
f(\lambda) = \frac{\langle \phi_i(\lambda) | \hat{n}_i | \phi_i(\lambda) \rangle}{\| \phi_i(\lambda) \|^2} + \frac{\langle \phi_{i+1}(\lambda) | \hat{n}_{i+1} | \phi_{i+1}(\lambda) \rangle}{\| \phi_{i+1}(\lambda) \|^2} = \langle \Psi_i | \hat{n}_i | \Psi_i \rangle + \langle \Psi_{i+1} | \hat{n}_{i+1} | \Psi_{i+1} \rangle. \tag{20}
\]

Thus the normalized states

\[
|\Phi_i^{(j+1)}\rangle = |\phi_i(\lambda^*)\rangle, \quad |\Phi_{i+1}^{(j+1)}\rangle = |\phi_{i+1}(\lambda^*)\rangle. \tag{21}
\]

preserve \( \langle \hat{n}_i + \hat{n}_{i+1} \rangle \) (Eq. 14) and are a rank-1 approximation of the evolved two-site state \( \tilde{U} |\Psi_i\rangle |\Psi_{i+1}\rangle \).

We cannot prove in general that the sequence of states just defined converges to the solution of Eqs. (14), (15), (16) and (17), but we have observed that this is always the case when \( \mathcal{U} \) is a unitary operator close to the identity as in TDMRG simulations. In this case, one can linearize \( f(\lambda) \) in \( \lambda = 0 \) and obtain a very good guess for the solution of Eq. (20) \( \Delta \hat{n}_i = \hat{n}_i - \langle \hat{n}_i \rangle \)

\[
\lambda_{\text{guess}} = -\frac{1}{2} \frac{\langle \phi_i(0) | \hat{n}_i | \phi_i(0) \rangle + \langle \phi_{i+1}(0) | \hat{n}_{i+1} | \phi_{i+1}(0) \rangle - \langle \Psi_i | \hat{n}_i | \Psi_i \rangle - \langle \Psi_{i+1} | \hat{n}_{i+1} | \Psi_{i+1} \rangle}{\langle \phi_i(0) | (\Delta \hat{n}_i)^2 | \phi_i(0) \rangle + \langle \phi_{i+1}(0) | (\Delta \hat{n}_{i+1})^2 | \phi_{i+1}(0) \rangle}. \tag{22}
\]

In our simulations we always found that \( \lambda^* \in [0, 2\lambda_{\text{guess}}] \) and that convergence is achieved in \( \lesssim 5 \) steps. In Fig. 3 we show a test of the algorithm just presented against a much more numerically demanding simulation performed using a number-conserving MPS. The density profile \( n_i \) is shown after quenching a complex hopping term \(-J \sum_i \left( e^{i \phi(t)} \hat{a}_i^\dagger \hat{b}_{i+1} + e^{-i \phi(t)} \hat{a}_{i+1}^\dagger \hat{b}_i \right)\) from \( \phi(t = 0) = 0 \) to \( \phi(t > 0) = 0.05 \) in the Hamiltonian (1) with \( U/J = 1.0 \). This amounts to a finite momentum delivered to the system. This kind of quench has been studied in Ref. 32 and 33.

The \( \mu \)-GVW evolved with the corrected TDMRG algorithm is able to capture the main features of the 1D dynamics which is quite interesting given the drastic approximation. Clearly, the MPS result shows less pronounced density oscillations since quantum fluctuations are captured by the variational wavefunction contrary to the \( \mu \)-GVW, as discussed in Sec. IV and in the caption of Fig. 1. The inset of Fig. 3 shows that without the correction the simulations are not reliable since \( \langle \hat{N} \rangle \) decreases rapidly in time producing wrong results.

V. CONCLUSIONS

In summary, we have shown that the common grand-canonical and number-conserving Gutzwiller Ansätze are simply the zero-order approximation of an expansion in
the truncation parameter $\epsilon$ of a Matrix Product State (MPS). This is an alternative point of view with respect to Ref. 34 where the GVW can be derived as a saddle point approximation of an appropriate functional integral. Moreover, although equally efficient from a computational point of view, we have explicitly shown that a number-conserving GVW is less efficient in capturing the ground state of a quantum system than a more general MPS. We believe that this is an important point to make since, despite the crudeness of the approximation, the Gutzwiller wavefunction is still a workhorse for the study of correlation effects in quantum systems, and it may be possible that even in higher dimensions a more general MPS (or PEPS in this case) of a relatively small and manageable size provides better results.

On the other hand, since the GVW can be easily applied to correlated quantum systems in higher dimensions – and indeed the approximation improves with increasing dimension –, we have suggested a novel time-evolution algorithm to exactly conserve the expectation value of the number of particles when a GVW or a MPS are not explicitly number-conserving. This algorithm can find application in one dimension for MPSs, and in dimensions higher than one for the GVW. Most importantly, we have found that the GVW dynamics obtained with our algorithm compares very well with the exact one in 1D. As subsequent projects it would then be of great interest to apply our algorithm to correlated quantum systems in higher dimensions and compare with experiments or other theoretical methods such as DMFT or LDA+U approximation schemes.

ACKNOWLEDGMENTS

This work has been supported by DOE under Grant No. DE-FG02-05ER46204. The Gutzwiller code developed for this work is made available at Ref. 31. The TDMRG code based on MPS has been developed in collaboration with Davide Rossini at the Scuola Normale Superiore, Pisa (Italy).

1 M. C. Gutzwiller, Phys. Rev. Lett. 10, 159 (1963).
2 J. Bünemann, W. Weber and F. Gebhard, Phys. Rev. B 57, 6896 (1998).
3 J. Hubbard, Proc. R. Soc. London A 276, 238 (1963).
4 J. Kanamori, Prog. Theor. Phys. 30, 275 (1963).
5 G. Borghi, M. Fabrizio, E. Tosatti, arXiv:1307.5738.
6 D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. 81, 3108 (1998).
7 P. W. Anderson, Science 235, 1196 (1987).
8 F. C. Zhang, C. Gros, T. M. Rice H. Shiba, Supercond. Sci. Technol. 1, 36 (1988).
9 B. Edegger, V. N. Muthukumar, C. Gros, Adv. Phys. 56, 927 (2007).
10 A. B. Bernevig, R. B. Laughlin, David I. Santiago, Phys. Rev. Lett. 97, 147003 (2003).
11 J. Bünemann, Florian Gebhard, R. Thul, Phys. Rev. B 67, 075103 (2003).
12 J. Bünemann, F. Gebhart, T. Ohm, S. Weiser, W. Weber, Phys. Rev. Lett. 101, 236404 (2008).
13 S. Östlund and S. Rommer, Phys. Rev. Lett. 75, 3537 (1995).
14 S. R. White, Phys. Rev. Lett. 69, 2863 (1992).
15 S. R. White, Phys. Rev. B 48, 10345 (1993).
16 U. Schollwöck, Ann. Phys. (NY) 326, 96 (2011).
17 E. M. Stoudenmire, S. R. White, Annual Review of Condensed Matter Physics 3, 111 (2012).
18 F. Verstraete, J. I. Cirac, arXiv:cond-mat/0407066.
19 T. Nishino, Y. Hieida, K. Okumishi, N. Maeshima, Y. Akutsu, A. Gendiar, Prog. Theor. Phys. 105, 409 (2001).
20 S. R. White, A. E. Feiguin, Phys. Rev. Lett. 93, 076401 (2004).
21 Guifré Vidal, Phys. Rev. Lett. 93, 040502 (2004).
22 A. J. Daley, C. Kollath, U. Schollwöck and G. Vidal, J. Stat. Mech. (2004) P04005.
23 D. Jaksch, V. Venturi, J. I. Cirac, C. J. Williams, P. Zoller, Phys. Rev. Lett. 89, 040402 (2002).
24 M. Snoek, W. Hofstetter, Phys. Rev. A 76, 051603(R) (2007).
25 J. Wernsdorfer, Michiel Snoek, Walter Hofstetter, Phys. Rev. A 81, 043620 (2010).
26 S. S. Natu, K. R. A. Hazzard, E. J. Mueller, Phys. Rev. Lett. 106, 125301 (2011).
27 J.-S. Bernier, D. Poletti, P. BarnettG, G. Roux, C. Kollath, Phys. Rev. A85, 033641 (2012).
28 M. P. A. Fisher, P. B. Weichman, G. Grinstein, Daniel S. Fisher, Phys. Rev. B40, 546 (1989).
29 Wilhelm Zwerger, J. Opt. B: Quantum Semiclass. Opt 5, S9 (2003).
30 T. Kühner et al., Phys. Rev. B61, 12474 (2000).
31 A working Python implementation is available at http://physics.ucsd.edu/~speotta/nuggetz.html.
32 S. Peotta, C.-C. Chen, M. Di Ventra, to be published.
33 C.-C. Chien M. Di Ventra, Phys. Rev. A87, 023609 (2013).
34 G. Kotliar, A. E. Ruckenstein, Phys. Rev. Lett. 57, 1362 (1986).