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Non-Stochastic Algorithms for Jastrow-Slater and Correlator Product State Wavefunctions

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Jastrow-Slater and correlator product state wavefunctions, two classes of quantum many-body wavefunctions, are commonly studied using Monte Carlo methods with the associated drawbacks of stochastic error. Here we show that efficient non-stochastic algorithms for these wavefunctions exist, both for observable evaluation and for optimization. The algorithms rely on the structure of these states as a product of local, commuting, invertible operators acting on a simple reference wavefunction. We describe the non-stochastic energy evaluation and optimization algorithms, and demonstrate them with applications to the Heisenberg and spinless and full Hubbard models. Our results demonstrate that the non-stochastic algorithms yield optimized wavefunctions and energies very close to those obtained with the variational Monte Carlo algorithm. Such algorithms provide new criteria for identifying new classes of wavefunctions for efficient computational simulation.

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I. INTRODUCTION

Explicit wavefunction approximations present a powerful approach to understanding the behavior of quantum many-body systems. For a wavefunction to be computationally useful, it is not sufficient to simply have a compact form. Instead it must also be possible to efficiently evaluate expectation values. Expectation values formally involve a trace over the Hilbert space which is of exponential dimension. The evaluation of this trace can often be carried out efficiently with Monte Carlo techniques. However, this introduces statistical error which must be controlled and which can lead to certain complications, for example in wavefunction optimization.

The Jastrow-Slater wavefunction^{1,2} is one of the most common wavefunctions used together with Monte Carlo sampling in fermionic systems. As the name suggests, the wavefunction augments a Slater determinant, the appropriate state for a system of non-interacting fermions, with a set of Jastrow factors. Jastrow factors are diagonal operators in the lattice basis and can be thought of as directly introducing correlations between particles in the system. Jastrow-Slater wavefunctions also form the starting point for more flexible wavefunctions such as the Jastrow-Antisymmetrized Geminal Power³⁻⁵ and Jastrow-Bardeen-Cooper-Schrieffer⁶ wavefunctions.

Recently, a second class of wavefunctions, termed correlator product states (CPS)⁷, entangled plaquette states (EPS)^{8,9}, or complete graph tensor networks¹⁰, have also been studied with Monte Carlo methods. We refer to these wavefunctions collectively as correlator product states here. These wavefunctions were constructed as a way to generalize the density matrix renormalization group (DMRG)^{11,12} to higher dimensions, while avoiding the computational cost of recent classes of tensor network wavefunctions such as the projected entangled pair states (PEPS)¹³⁻²³ or multiscale entanglement renormalization ansatz (MERA)^{24,25}. The correlator product state directly approximates a wavefunction as a product of correlator amplitudes. Correlators are diagonal operators, and are thus mathematically identical to Jastrow factors. Consequently the correlator product state is also a pure Jastrow wavefunction. In this work the term correlator will be used to refer to both correlators as used in the CPS, and the Jastrow factors used in the Jastrow-Slater wavefunction.

While the form of the Jastrow-Slater and CPS wavefunctions make them a natural fit for Monte Carlo algorithms, it is interesting to ask whether or not statistical algorithms, with their associated drawbacks of statistical error, are the only way to manipulate these states. Here we will show that efficient non-stochastic algorithms exist both to evaluate observables and to optimize the CPS and Jastrow-Slater wavefunction, so long as we are willing to sacrifice the strict variational principle. The non-stochastic algorithms rely on the common structure of the Jastrow-Slater and CPS wavefunctions, namely that they are a product of local, commuting, invertible operators acting on a simple reference state. Other wavefunctions, such as the coupled cluster wavefunction, also take this form, and the algorithms we describe are similar to the techniques used for observable evaluation and wavefunction optimization in the coupled cluster literature²⁶.

As we shall see, the non-stochastic methodology we employ can be written in terms of a similarity transform on the Hamiltonian that attempts to convert the system of correlated physical particles into a system of weakly correlated or uncorrelated quasi particles. In this respect our approach shares many similarities with a number of other methods, in particular the transcorrelated wave equation (TWE)²⁷, the method of correlated basis functions (CBF)²⁸, and coupled cluster theory. In each of these methods, as well as in our own, one must limit the form of the modified Hamiltonian and possibly introduce other approximations in order to achieve computational feasibility. It is the nature of these limitations and approximations that differentiate these methods. In the TWE, the correlating factor (which here we would refer to as a correlator or Jastrow factor) is limited to correlating no more than two particles at a time, allowing one to evaluate the necessary integrals by numerical quadrature. In the CBF approach, the variational energy expression is simplified through a perturbatively motivated truncation based on the ratio of the (supposedly small) volume in which two particles correlate to the total volume of the system, and the resulting expression is minimized using a linear combination of determinants rather than a single determinant. Our approach also uses the concept of a small correlation volume, but not in a perturbative manner. Instead, we explicitly limit the range over which our “correlating functions” (correlators or Jastrow factors) can operate, which makes the complexity of the operators in the similarity transformed Hamiltonian independent of system size. Unlike the TWE and CBF methods, our method permits the use of many-body (i.e. more than two-body) correlation functions, which is critical when working with CPS tensor networks. Finally, coupled cluster theory uses an approach that is mathematically very similar to ours, although there the form of the correlating function is different and the limitation is placed not on the range of the correlations in terms of real space distances but rather on the particle excitation rank relative to a reference state. To make a connection with the concept of locality, limiting the excitation rank in coupled cluster can be viewed as limiting the “energetic distance” from the reference.

We begin by reviewing the structure of the CPS and Jastrow wavefunctions (Sec. II A). We then proceed to describe the energy evaluation (Sec. II B) and optimization algorithms (Sec. II C). Demonstrations of these non-stochastic algorithms are carried out on the Heisenberg model (Sec. III A), the spinless Hubbard model (Sec. III B), and the full Hubbard model (Sec. III C). Our purpose in applying the method to these models is to establish the

validity of our approximations, and so in this study we have intentionally limited ourselves to systems for which the correct answers are more or less already known. After these lattice model tests, we finish with our conclusions in Sec. IV.

II. THEORY

A. The CPS and Jastrow-Slater Wavefunctions

Consider an arbitrary quantum wavefunction on k lattice sites. This can be written as

$$\begin{aligned} |\Psi\rangle &= \sum_{n_1 n_2 \dots n_k} \Psi_{n_1 n_2 \dots n_k} |n_1 n_2 \dots n_k\rangle \\ &= \sum_{\mathbf{n}} \Psi_{\mathbf{n}} |\mathbf{n}\rangle, \end{aligned} \quad (1)$$

where \mathbf{n} denotes the vector of occupancies $n_1 n_2 \dots n_k$. In a spin 1/2 system,

$$|n_i\rangle \in \{|\uparrow\rangle, |\downarrow\rangle\}, \quad (2)$$

while in a fermion system,

$$|n_i\rangle \in \{|-\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}. \quad (3)$$

Here, we describe the CPS and Jastrow-Slater approximations to $|\Psi\rangle$. We first define a Jastrow factor. A Jastrow factor is an operator that is diagonal in the lattice basis $|\mathbf{n}\rangle$. It is usually written as an exponential of an expansion in number operators,

$$\hat{J} = \exp(j + \sum_i j_i \hat{n}_i + \sum_{ij} j_{ij} \hat{n}_i \hat{n}_j + \dots). \quad (4)$$

In most applications, the Jastrow amplitudes $j, j_i, j_{ij} \dots$, are restricted to be real numbers, which makes the Jastrow factor \hat{J} positive definite. For full generality, however, we should regard the amplitudes as possibly being complex.

A correlator is also an operator that is diagonal in the lattice basis. It can be viewed as a Jastrow factor written in non-exponential form. A single correlator acts on a domain of sites. For example, a correlator on sites i, j takes the form

$$\begin{aligned} \hat{c}_{ij} &= \sum_{n_i n_j} |n_i n_j\rangle c_{n_i n_j} \langle n_i n_j| \\ &= \sum_{n_i n_j} c_{n_i n_j} \hat{P}_{n_i n_j}, \end{aligned} \quad (5)$$

where $c_{n_i n_j}$ are the correlator amplitudes, and we have introduced the projection operator $\hat{P}_{n_i n_j} = |n_i n_j\rangle \langle n_i n_j|$. The equivalence of the correlator and Jastrow factor is seen by recognizing that a two-site correlator \hat{c}_{ij} is exactly representable by a two-site Jastrow factor $\exp(j + j_i \hat{n}_i + j_{ij} \hat{n}_i \hat{n}_j)$, so long as the Jastrow amplitudes are allowed to be complex. The choice of using the exponentiated Jastrow representation or the correlator representation is a matter of numerical expediency. In the current work, we henceforth use the term “correlator” to refer to both representations.

A correlator can be chosen to act on an arbitrary number of sites (see Figs. 1 and 2). Such a general correlator is written as

$$\hat{c}_\lambda = \sum_{\mathbf{n}_\lambda} c_{\mathbf{n}_\lambda} \hat{P}_{\mathbf{n}_\lambda}, \quad (6)$$

where \mathbf{n}_λ is the occupancy vector of the sites in the domain of the correlator, and $\hat{P}_{\mathbf{n}_\lambda}$ is the corresponding projector.

Both Jastrow factors and correlators can be applied to reference wavefunctions $|\Phi\rangle$ to generate approximations to $|\Psi\rangle$. We start with the correlator product state (CPS). This is obtained from the uniform reference function $|\Phi_U\rangle$, an

equally weighted sum over the lattice quantum basis,

$$|\Phi_U\rangle = \sum_{\mathbf{n}} |\mathbf{n}\rangle. \quad (7)$$

The summation in Eq. (7) may be chosen with symmetry constraints. For example, in this work, we always use a uniform reference such that for spin systems, the summation in Eq. (7) refers to states only with given S_z , while for fermionic system, to states with only given N and given S_z .

The CPS is then obtained by applying a product of correlators to $|\Phi_U\rangle$,

$$|\Psi\rangle = \hat{C}|\Phi_U\rangle = \prod_{\lambda} \hat{c}_{\lambda}|\Phi_U\rangle. \quad (8)$$

The correlator amplitudes $c_{\mathbf{n}_{\lambda}}$ provide a product approximation to the wavefunction amplitudes $\Psi_{\mathbf{n}}$ in Eq. (1)

$$\Psi_{\mathbf{n}} = \prod_{\lambda} c_{\mathbf{n}_{\lambda}}, \quad (9)$$

and this expression can be evaluated efficiently in a time proportional to the number of correlators. Note that the domains λ of the different correlators will usually contain overlapping sites. For example, for a CPS wavefunction in one-dimension with nearest neighbor correlators, we have

$$|\Psi\rangle = \hat{c}_{12}\hat{c}_{23}\hat{c}_{34}\dots\hat{c}_{k-1k}|\Phi_U\rangle. \quad (10)$$

By using correlators that cover increasingly larger numbers of sites, CPS become an exact family of states.

The Jastrow-Slater fermion wavefunction is obtained by applying a set of correlators (i.e. Jastrow factors) to a Slater determinant reference of orbitals $|\Phi_D\rangle = \det|\phi_1\phi_2\dots\phi_N|$,

$$|\Psi\rangle = \hat{C}|\Phi_D\rangle. \quad (11)$$

The wavefunction amplitudes in this case are given by

$$\Psi_{n_1 n_2 \dots n_k} = \prod_{\lambda} c_{\mathbf{n}_{\lambda}} \times \det|\phi_1(r_1)\phi_2(r_2)\dots\phi_N(r_N)|, \quad (12)$$

where $r_1, r_2 \dots r_N$ label the positions of the N sites occupied in the occupancy vector $|n_1 n_2 \dots n_k\rangle$. The determinant contribution to the wavefunction amplitude can be evaluated efficiently in $O(N^3)$ time. As in the case of the CPS, Jastrow-Slater wavefunctions become an exactly family of states if the correlators (Jastrows) cover larger and larger numbers of sites.

Both the CPS and Jastrow-Slater wavefunctions have so far been used in conjunction with Monte Carlo algorithms. In variational Monte Carlo^{29,30}, the energy is written as

$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_{\mathbf{n}} \frac{|\Psi_{\mathbf{n}}|^2}{\langle\Psi|\Psi\rangle} E_L(\mathbf{n}), \quad (13)$$

where the local energy $E_L(\mathbf{n})$ is defined by

$$E_L(\mathbf{n}) = \sum_{\mathbf{n}'} \frac{\Psi_{\mathbf{n}'}}{\Psi_{\mathbf{n}}} \langle\mathbf{n}|H|\mathbf{n}'\rangle. \quad (14)$$

As long as $\Psi_{\mathbf{n}}$ can be evaluated efficiently, which is the case for both the CPS and Jastrow-Slater wavefunctions, a Markov chain can be used to sample the probability distribution $|\Psi_{\mathbf{n}}|^2/\langle\Psi|\Psi\rangle$ and to efficiently compute the overall energy as an average of the sampled local energies. The wavefunctions may also be variationally optimized using stochastic estimates for the gradient of the energy with respect to the wavefunction amplitudes. Variational Monte Carlo is a stochastic approach to using the CPS and Jastrow-Slater wavefunctions. A disadvantage of stochastic algorithms is the presence of statistical error, which must be controlled by increasing the sample size. We now show how statistical noise can be avoided by using non-stochastic algorithms both to evaluate the energy of, and to optimize the amplitudes of, CPS and Jastrow-Slater wavefunctions.

B. Non-Stochastic Energy Evaluation

The idea behind our approach to non-stochastic energy evaluation is the following. First, we assume that the CPS or Jastrow wavefunction $|\Psi\rangle = \hat{C}|\Phi\rangle$ (we use $|\Phi\rangle$ to refer to either the uniform or determinant reference) is an eigenstate of the Hamiltonian H ,

$$H\hat{C}|\Phi\rangle = E\hat{C}|\Phi\rangle. \quad (15)$$

The energy is then obtained as the asymmetric expectation value

$$E = \langle\Phi|\hat{C}^{-1}H\hat{C}|\Phi\rangle = \langle\Phi|\bar{H}|\Phi\rangle, \quad (16)$$

where we define the similarity transformed effective Hamiltonian, $\bar{H} = \hat{C}^{-1}H\hat{C}$.

Efficient non-stochastic energy evaluation now reduces to whether or not $\langle\bar{H}\rangle$ can be efficiently obtained with the reference state $|\Phi\rangle$, where $|\Phi\rangle$ is a uniform reference in the case of CPS, or a determinant in the case of the Jastrow-Slater wavefunction. By efficient, we mean that the cost is polynomial in the lattice size. The standard expectation value $\langle\Phi|H|\Phi\rangle$ can be efficiently evaluated in either case because the individual terms in the Hamiltonian act on a small number of sites, independent of lattice size. For example, the Heisenberg and Hubbard Hamiltonians contain terms which only act at most on a pair of sites. The corresponding terms in the effective Hamiltonian \bar{H} act on a larger number of sites due to the similarity transformation by the correlators. However, if the size and range of the correlators are independent of lattice size, then even after similarity transformation, the terms in \bar{H} still act on a number of sites that will be independent of lattice size. Consequently, the expectation value $\langle\bar{H}\rangle$ can still be evaluated at a cost scaling polynomially with respect to the lattice size. As we shall see, the magnitude of the evaluation cost (although not its scaling with respect to system size) is strongly dependent on the range of the correlators. One of the questions we seek to answer in this work is what the practical limits for correlator range are and what accuracy can be achieved within these limits.

For a more concrete view of the non-stochastic energy evaluation, consider the energy contribution E_{xy} from a hopping operator $a_x^\dagger a_y$ associated with sites x and y ,

$$E_{xy} = \langle\Phi|\hat{C}^{-1}a_x^\dagger a_y\hat{C}|\Phi\rangle. \quad (17)$$

We can divide the correlators in \hat{C} (and their inverses in \hat{C}^{-1}) into two classes: those which involve (touch) sites x or y and those which do not. Denote the product of all the correlators which involve x or y as \hat{C}_{xy} , and the product of the remaining correlators as $\hat{C}_{\overline{xy}}$. Then we have

$$\hat{C} = \hat{C}_{xy} \hat{C}_{\overline{xy}}. \quad (18)$$

As an example, consider the hopping operator $a_3^\dagger a_4$, and the one dimensional CPS in Eq. (10). Then, \hat{C}_{34} is given by

$$\hat{C}_{34} = \hat{c}_{23}\hat{c}_{34}\hat{c}_{45}. \quad (19)$$

Because $\hat{C}_{\overline{xy}}$ only contains correlators which do *not* involve sites x or y , it can be commuted past $a_x^\dagger a_y$ in Eq. (17) to cancel with its corresponding inverse $\hat{C}_{\overline{xy}}^{-1}$,

$$\begin{aligned} E_{xy} &= \langle\Phi|\hat{C}_{xy}^{-1} \hat{C}_{\overline{xy}}^{-1} a_x^\dagger a_y \hat{C}_{xy} \hat{C}_{\overline{xy}}|\Phi\rangle \\ &= \langle\Phi|\hat{C}_{xy}^{-1} a_x^\dagger a_y \hat{C}_{xy}|\Phi\rangle. \end{aligned} \quad (20)$$

Thus, the similarity transform of $a_x^\dagger a_y$ involves only \hat{C}_{xy} , not the whole \hat{C} operator. The correlators in \hat{C}_{xy} define a cluster of k_{xy} sites, where the size depends on the sizes and ranges of the correlators and the geometry of the cluster, but is independent of lattice size as long as the correlators are local. The transformed hopping operator $\hat{C}_{xy}^{-1} a_x^\dagger a_y \hat{C}_{xy}$ now acts on k_{xy} sites. The energy contribution E_{xy} thus requires evaluating the expectation value of a k_{xy} site operator with the reference function $|\Phi\rangle$.

To see the explicit dependence of the evaluation of $\langle a_x^\dagger a_y \rangle$ on the reference function, we separate \hat{C}_{xy} into its

amplitude and projection operator components

$$\hat{C}_{xy} = \sum_{\mathbf{n}_{xy}} C_{\mathbf{n}_{xy}} \hat{P}_{\mathbf{n}_{xy}}, \quad (21)$$

where \mathbf{n}_{xy} is the occupancy vector for the cluster of sites defined by \hat{C}_{xy} . The expectation values of the projection operators define a many-body reduced density-matrix (RDM) γ on k_{xy} sites

$$\gamma_{\mathbf{n}_{xy}, \mathbf{n}'_{xy}} = \langle \Phi | \hat{P}_{\mathbf{n}_{xy}} a_x^\dagger a_y \hat{P}_{\mathbf{n}'_{xy}} | \Phi \rangle. \quad (22)$$

The evaluation of γ depends on the form of the reference function $|\Phi\rangle$. In the case of the CPS, each element of the RDM is obtained in $O(1)$ time (even with particle number and S_z restrictions). For a Jastrow-Slater wavefunction, the corresponding RDM element can be evaluated as a determinant of one-body RDM elements in $O(k_{xy}^3)$ time. Once the RDM is obtained, the combination with the amplitudes is independent of the reference. The expectation value E_{xy} becomes

$$E_{xy} = \sum_{\mathbf{n}_{xy} \mathbf{n}'_{xy}} C_{\mathbf{n}_{xy}}^{-1} \gamma_{\mathbf{n}_{xy}, \mathbf{n}'_{xy}} C_{\mathbf{n}'_{xy}}. \quad (23)$$

Due to the summation over the occupancy vector, the cost of Eq. (23) is exponential in the cluster size, k_{xy} , but not in the lattice size. Note that the cost is effectively the cost of a single summation over \mathbf{n}_{xy} , rather than the formal double summation shown above, because the sparsity of γ means that it has $O(d^{k_{xy}})$ non-zero elements, where d is dimension of a single site. For sufficiently short-range correlators, which lead to small clusters, the summation can be carried out affordably. As each operator in the Hamiltonian involves a similar contribution, the entire energy may be efficiently evaluated.

The non-stochastic energy evaluation algorithm relies on little of the detailed structure of the Jastrow-Slater and CPS wavefunctions. The key steps require only that (i) \hat{C} is made of a product of local, commuting, invertible operators, (ii) only a small number of these operators do not commute with a given term in the Hamiltonian, and (iii) the reference function $|\Phi\rangle$ is sufficiently simple that the expectation values in Eq. (22) can be efficiently obtained. This structure is obeyed by many other wavefunctions, such as the coupled cluster wavefunction²⁶ (although there locality refers to the particle rank of excitations out of some reference function rather than a distance in real space), and indeed for any wavefunction with this structure, an efficient non-stochastic energy evaluation algorithm may be formulated.

C. Non-Stochastic Wavefunction Optimization

Above we showed that we can evaluate the approximate energy of a CPS or Jastrow-Slater wavefunction in a non-stochastic way, as long as the individual correlators or Jastrow factors do not cover too many sites. For a complete calculation, we need to also determine the correlator or Jastrow amplitudes. Since the non-stochastic energy is not variational, we cannot obtain the optimal parameters by a minimization of the energy. Instead, we require that the CPS or Jastrow wavefunction satisfies a set of non-linear projected Schrödinger equations. Solving these equations yields exactly the same solution as the minimum of the variational energy if the wavefunction provides an exact parameterization, although this is not the case for approximate CPS and Jastrow wavefunctions.

As in the previous section, we assume that the CPS or Jastrow wavefunction is a true eigenstate of the Hamiltonian, Eq. (15). From the Schrödinger equation, we need to obtain a set of non-linear equations equal in number to the number of amplitudes in \hat{C} . We obtain sufficient equations by projecting with the bras $\langle \Phi | \hat{P}_{\mathbf{n}_\lambda}$, where $\hat{P}_{\mathbf{n}_\lambda}$ are the projectors used to define the correlator operators in Eq. (6). Applying these bra states gives us

$$\langle \Phi | \hat{P}_{\mathbf{n}_\lambda} (\hat{H} - E) | \Phi \rangle = R_{\mathbf{n}_\lambda} = 0. \quad (24)$$

By requiring the residuals $R_{\mathbf{n}_\lambda}$ to vanish we determine all the correlator amplitudes $c_{\mathbf{n}_\lambda}$. As with energy evaluation, the expectation value in Eq. (24) can be obtained in a non-stochastic manner by tracing over clusters of sites associated with each similarity transformed term in the effective Hamiltonian \bar{H} .

In order to solve the simultaneous set of equations (24), we have taken two approaches. In the first case, we use a standard Newton-Raphson procedure to find the simultaneous zeroes of the residuals $R_{\mathbf{n}_\lambda}$. This requires evaluating the Jacobian matrix $\partial R_{\mathbf{n}_\lambda} / \partial c_{\mathbf{n}_\mu}$. Alternatively, we may take the approach of constructing and diagonalizing a local Hamiltonian for each correlator's amplitudes. The local Hamiltonian and overlap matrices that determine $c_{\mathbf{n}_\lambda}$ are

defined as

$$\bar{H}_{\mathbf{n}_\lambda, \mathbf{n}'_\lambda} = \langle \Phi | \hat{P}_{\mathbf{n}_\lambda} c_{\mathbf{n}_\lambda} \bar{H} c_{\mathbf{n}'_\lambda}^{-1} \hat{P}_{\mathbf{n}'_\lambda} | \Phi \rangle, \quad (25)$$

$$S_{\mathbf{n}_\lambda, \mathbf{n}'_\lambda} = \langle \Phi | \hat{P}_{\mathbf{n}_\lambda} \hat{P}_{\mathbf{n}'_\lambda} | \Phi \rangle. \quad (26)$$

The correlator amplitudes are obtained from solving an eigenvalue problem for each correlator \hat{c}_λ ,

$$\sum_{\mathbf{n}'_\lambda} \bar{H}_{\mathbf{n}_\lambda, \mathbf{n}'_\lambda} c_{\mathbf{n}'_\lambda} = E \sum_{\mathbf{n}'_\lambda} S_{\mathbf{n}_\lambda, \mathbf{n}'_\lambda} c_{\mathbf{n}'_\lambda}. \quad (27)$$

The local Hamiltonian matrix $\bar{H}_{\mathbf{n}_\lambda, \mathbf{n}'_\lambda}$ depends on the amplitudes of all the correlators, $\hat{c}_{\mu \neq \lambda}$. Thus after each correlator amplitude is obtained from the respective eigenvalue problem (27), the local Hamiltonians are updated, and the procedure is iterated until convergence is achieved.

Much as in the case of energy evaluation, the formulation of the amplitude equations relies only on generic elements of the product structure of the Jastrow-Slater and CPS wavefunctions. By analogy with methods for the coupled cluster wavefunction, we can also write down a non-stochastic algorithm to obtain expectation values of arbitrary operators. Starting from the amplitude equations, we first define a Lagrangian as

$$L = \langle \Phi | \bar{H} + \sum_{\mathbf{n}_\mu} \Lambda_{\mathbf{n}_\mu} \hat{P}_{\mathbf{n}_\mu} (\bar{H} - \langle \Phi | \bar{H} | \Phi \rangle) | \Phi \rangle, \quad (28)$$

from which the amplitude equations arise from the stationary conditions

$$\frac{\partial L}{\partial \Lambda_{\mathbf{n}_\mu}} = 0. \quad (29)$$

The values of the Lagrange multipliers $\Lambda_{\mathbf{n}_\mu}$ are found by requiring the Lagrangian to be stationary with respect to the correlator variables $c_{\mathbf{n}_\mu}$,

$$\frac{\partial L}{\partial c_{\mathbf{n}_\mu}} = 0. \quad (30)$$

Then, derivatives of the Lagrangian with respect to the Hamiltonian's parameters define reduced density matrices as

$$\Gamma_{ij} = \langle \Phi | \overline{a_i^\dagger a_j} + \sum_{\mathbf{n}_\mu} \Lambda_{\mathbf{n}_\mu} \hat{P}_{\mathbf{n}_\mu} \left(\overline{a_i^\dagger a_j} - \langle \Phi | \overline{a_i^\dagger a_j} | \Phi \rangle \right) | \Phi \rangle, \quad (31)$$

where $\overline{a_i^\dagger a_j} = \hat{C}^{-1} a_i^\dagger a_j \hat{C}$. The two body reduced density matrix Γ_{ijkl} is defined likewise using $\overline{a_i^\dagger a_j^\dagger a_l a_k}$. These density matrices allow us to obtain expectation values of arbitrary one and two body operators.

III. RESULTS

In this section we report results for a number of benchmark calculations in which we test the assumptions inherent to our non-stochastic approach. It is not within the scope of our study to investigate new phenomena with our technique. Instead we limit ourselves to systems for which the correct results are more or less known in order to assess the performance of our approach. To simplify the tabulation of data, we have used the abbreviations NS (non-stochastic energy of the non-stochastic wavefunction), VNS (variational energy of the non-stochastic wavefunction), and %D (percent difference from the variational energy of the variational wavefunction). Where appropriate, we include the statistical uncertainty of the final digit in parentheses.

A. Antiferromagnetic Heisenberg Model

We have applied the correlator product state to the antiferromagnetic spin- $\frac{1}{2}$ Heisenberg model on a periodic 8x8 square lattice and a periodic 6x6 triangular lattice using both the non-stochastic and variational MC frameworks.

The Hamiltonian is written as

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j, \quad (32)$$

where $\langle ij \rangle$ indicates nearest neighbor pairs and $J > 0$. The results are summarized in Tables I and II. In the case of the square lattice, we have essentially exact stochastic series expansion (SSE) results with which to compare³¹. While the accuracy of the CPS ansatz is not the main question we are studying here (such studies can be found in Refs.⁷⁻⁹), we see that both the non-stochastic and variational Monte Carlo energies are within 2% of the SSE result for 4-site square correlators and about 1% for 9-site square correlators. The more central question here is the relative difference between the non-stochastic and variational Monte Carlo energies. We see that in all cases, the relative difference is comparable to the intrinsic energy error associated with the wavefunction, and in one case it is significantly smaller. As a measure of the variational quality of the non-stochastic results, we have also computed the variational energy of the wavefunctions resulting from our non-stochastic optimization (to save space in tabulation we term this the VNS energy). We see that in most cases that this energy is very similar to the minimal variational energy, especially in the case of the largest correlators (9-site squares and 7-site hexagons).

As expected, the non-stochastic energy is not variational, and for small correlators it tends to be slightly below the variational energy. More surprisingly, the convergence in accuracy for the non-stochastic energy is not monotonic with correlator size. We see both larger deviations from the variational Monte Carlo results, as well as lower accuracy in the total energy, for 5-site crosses (in the square lattice) and 6-site triangles (in the triangular lattice), than for some smaller correlators. We find that square and rhombus correlators do particularly well on the square and triangular lattices, respectively, with relative differences from the variational energy all within 1%. We speculate that these correlators' success is due in part to the fact that the amplitude equations used in their optimization (Eq. (24)) are constructed using projectors that share the translational symmetry of the underlying lattice.

One appealing aspect of the non-stochastic method for CPS on periodic spin lattices is that the cost of the method can be made independent of the lattice size by using translationally invariant correlators and by taking advantage of the uniform reference's particularly simple RDM elements (Eq. (22)). As seen in Table VI, the non-stochastic method was much faster than variational MC for small correlators (5-site crosses/4-site rhombuses and smaller), while being slower for larger correlators due to the exponential increase of the cost with correlator size.

B. Spinless Hubbard Model

We have studied a 20-site (4x5) spinless Hubbard lattice with open boundary conditions using the Jastrow-Slater wavefunction and the non-stochastic algorithms. We have also performed variational Monte Carlo calculations for comparison. While we could treat much larger lattices, we chose this lattice size in order to compare to exact results. The Hamiltonian for the spinless Hubbard model is

$$H = \sum_{\langle ij \rangle} -t(a_i^\dagger a_j + a_j^\dagger a_i) + U a_i^\dagger a_i a_j^\dagger a_j, \quad (33)$$

in which a_i^\dagger and a_i are the fermionic particle creation and destruction operators on site i , and $\langle ij \rangle$ represents nearest neighbors.

Results for half-filling and single hole doping are presented in Figs. 3 and 4 and Tables III and IV, respectively. We find that the difference between the non-stochastic and variational Monte Carlo energies is small for all ratios of U/t at both half-filling and single hole doping. At half-filling, the largest difference is 0.06%, while for single hole doping, it is 0.18%. The energy errors of the Jastrow-Slater form (compared to the exact energy) are less than 1% for all values of U/t at half-filling, and below 3% for single hole doping. We see that the difference between the non-stochastic and variational Monte Carlo energies is here much smaller than the intrinsic error associated with the quality of the wavefunction.

C. Full Hubbard Model

We have also studied the Hubbard model at half filling with open boundary conditions, in one and two dimensions, using the non-stochastic and variational Monte Carlo algorithms for the Jastrow-Slater wavefunction. The Hubbard

Hamiltonian is

$$H = -t \sum_{\langle ij \rangle} \sum_{\sigma=\uparrow,\downarrow} (a_{i\sigma}^\dagger a_{j\sigma} + a_{j\sigma}^\dagger a_{i\sigma}) + U \sum_i a_{i\uparrow}^\dagger a_{i\uparrow} a_{i\downarrow}^\dagger a_{i\downarrow}, \quad (34)$$

in which $a_{i\uparrow(\downarrow)}^\dagger$ and $a_{i\uparrow(\downarrow)}$ are the fermionic creation and destruction operators for particles with spin \uparrow (\downarrow), and $\langle ij \rangle$ refers to nearest neighbors.

Since the fermions have spin, there are several choices of Slater determinant possible. We use as our Slater determinant the restricted Hartree-Fock (RHF) Slater determinant. While better energies could be obtained with an unrestricted or generalized Slater determinant, the restricted Hartree-Fock determinant is sufficient for the comparison between the non-stochastic and variational Monte Carlo algorithms that is our primary concern.

Results for the ratios $U/t = 2$ and $U/t = 4$ are presented in Table V. For $U/t = 2$, the bare RHF Slater determinant produces energies in error by 6-10%, which are reduced to 1% or less after the inclusion of Jastrow factors, optimized either through the non-stochastic or variational Monte Carlo algorithms. Importantly, the non-stochastic energies lie within the error bars of the variational CPS energies for both the one and two dimensional lattices. For the case of $U/t = 4$, the RHF reference is qualitatively incorrect with relative errors as high as 60%. The inclusion of Jastrow factors reduces the error to 2% and 7% in one and two dimensions, respectively. Despite the poor quality of the wavefunction in this problem, the non-stochastic energy reproduces the variational CPS energy quite well, with the relative differences in Table V never exceeding 1%. This is much less than the intrinsic error due to the quality of the wavefunction.

As seen in Table VI, the cost of the non-stochastic method relative to variational Monte Carlo is less favorable than for the Heisenberg model. The reasons for this slowdown are twofold. First, the site dimension d is twice as large for the Hubbard model, and second, the evaluation of the RDM elements (while still polynomial scaling) is much higher for the Slater determinant than for the uniform reference. We note, however, that the cost scaling of the non-stochastic method is $O(N^2)$, while that of variational MC is $O(N^3)$ assuming that the number of samples needed grows linearly with system size. Thus for very large lattices, the non-stochastic approach may offer significant efficiencies.

Finally, for the 22-site chain with $U/t = 4$, we investigated the effect of varying the size of the Jastrow factor. As shown in Fig. 5, both the non-stochastic and variational energies improve when extending the Jastrow factor from one to four sites. We observe in all cases that the non-stochastic and variational energies differ by an amount significantly less than the intrinsic energy error of the wavefunction, except for the 4-site Jastrows, where the non-stochastic energy lies slightly below (-0.1%) below the true energy, while the variational energy is above (1.2%) and thus the difference between the non-stochastic and variational energies is almost exactly the same as the intrinsic variational energy error.

IV. CONCLUSIONS

We have shown that efficient non-stochastic algorithms exist both to evaluate the energy and expectation values of Jastrow-Slater and correlator product state wavefunctions, as well as to optimize the wavefunction parameters. We have tested our methods in three models: the spin- $\frac{1}{2}$ antiferromagnetic Heisenberg model, the spinless Hubbard model, and the full Hubbard model. While unlike the variational Monte Carlo energy, the non-stochastic energy is not a strict upper bound, the difference between the two energies is comparable to and often significantly less than the intrinsic error associated with the quality of the wavefunction. In practice we find that the non-stochastic algorithms are faster than the variational Monte Carlo algorithms for small correlator (or Jastrow) sizes, but become more expensive for larger correlators.

The non-stochastic algorithms we have described rely on the mathematical form of the Jastrow-Slater and correlator product state wavefunctions as a product of local, commuting, invertible operators acting on a simple reference wavefunction. Any wavefunction with this mathematical form may be studied with analogous efficient non-stochastic techniques. This possibility can guide the construction of efficient new classes of wavefunctions in the future.

V. ACKNOWLEDGMENTS

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TABLE I: Comparison of non-stochastic and variational MC results for the antiferromagnetic spin- $\frac{1}{2}$ Heisenberg model on the 8x8 square lattice with periodic boundary conditions and total $S_z = 0$. The energies per site are reported in units of J. The variational Monte Carlo error is reported relative to the essentially exact stochastic series expansion (SSE)³¹. Translationally invariant correlators are employed, with each of the two sublattices having independent correlators. When optimizing the correlators, Marshall's sign rule is used as an initial guess. The acronyms NS and VNS refer to the non-stochastic and variational energies, respectively, of the wavefunction resulting from a non-stochastic optimization, while %D indicates the percent difference between these energies and the variational energy of the VMC wavefunction.

Correlators	VMC	NS	%D	VNS	%D	VMC % Error
nearest neighbor	-0.6534(6)	-0.6883	-5.34	-0.6501(2)	0.51	2.98
4-site squares	-0.6617(3)	-0.6659	-0.64	-0.6561(2)	0.84	1.76
5-site crosses	-0.6637(3)	-0.6449	2.82	-0.6573(2)	0.97	1.46
9-site squares	-0.6699(2)	-0.6651	0.72	-0.6689(1)	0.15	0.53

TABLE II: Comparison of non-stochastic and variational MC results for the antiferromagnetic spin- $\frac{1}{2}$ Heisenberg model on the 6x6 triangular lattice with periodic boundary conditions and total $S_z = 0$. The energies per site are reported in units of J. Translationally invariant correlators are employed, with each of the three sublattices having independent correlators. When optimizing the correlators, the solution to the classical Heisenberg model is used as an initial guess. Here NS, VNS, and %D have the same meaning as in Table I.

Correlators	VMC	NS	%D	VNS	%D
nearest neighbor	-0.5184(2)	-0.5253	-1.33	-0.5183(1)	0.02
3-site triangles	-0.5184(2)	-0.5253	-1.33	-0.5183(1)	0.03
4-site rhombuses	-0.5383(3)	-0.5353	0.55	-0.5108(2)	5.11
6-site triangles	-0.5419(2)	-0.5289	2.40	-0.5353(1)	1.21
7-site hexagons	-0.5435(2)	-0.5390	0.83	-0.5397(1)	0.69

TABLE III: Total ground state energies, in units of t , for the 4×5 spinless Hubbard lattice at half filling with open boundary conditions. Both the non-stochastic and variational MC methods use 4-site square Jastrow factors (correlators). Exact results were computed using the sparse diagonalization routine in the ALPS program³². Here NS and %D have the same meaning as in Table I.

U / t	VMC	NS	%D	Hartree Fock	Exact
0.1	-13.8158(1)	-13.8157	0.00	-13.8117	-13.8166
0.2	-13.2438(2)	-13.2437	0.00	-13.2276	-13.2475
0.4	-12.1368(4)	-12.1367	0.00	-12.0709	-12.1544
0.6	-11.0611(2)	-11.0591	0.02	-10.9539	-11.1267
0.8	-10.0884(2)	-10.0850	0.03	-9.9598	-10.1737
1.0	-9.2273(2)	-9.2230	0.05	-9.0917	-9.3066
1.2	-8.4712(2)	-8.4660	0.06	-8.3382	-8.5326
1.4	-7.8072(2)	-7.8022	0.06	-7.6827	-7.8507
2.0	-6.2529(2)	-6.2491	0.06	-6.1622	-6.2658
4.0	-3.6141(1)	-3.6139	0.00	-3.5885	-3.6151
6.0	-2.4988(1)	-2.4989	-0.01	-2.4895	-2.4991
8.0	-1.9000(1)	-1.9007	-0.03	-1.8963	-1.9007
10.0	-1.5304(1)	-1.5308	-0.03	-1.5285	-1.5308

TABLE IV: Total ground state energies, in units of t , for the 4×5 spinless Hubbard lattice with single hole doping and open boundary conditions. Both the non-stochastic and variational MC methods use 4-site square Jastrow factors (correlators). Exact results were computed using the sparse diagonalization routine in the ALPS program³². Here NS and %D have the same meaning as in Table I.

U / t	VMC	NS	%D	Hartree Fock	Exact
0.1	-13.8554(1)	-13.8554	0.00	-13.8522	-13.8558
0.2	-13.4339(1)	-13.4341	0.00	-13.4214	-13.4359
0.4	-12.6194(4)	-12.6195	0.00	-12.5685	-12.6268
0.6	-11.8411(2)	-11.8410	0.00	-11.7262	-11.8583
0.8	-11.0985(3)	-11.0976	0.01	-10.8940	-11.1303
1.0	-10.3921(3)	-10.3886	0.03	-10.0718	-10.4434
1.2	-9.6579(4)	-9.6456	0.13	-9.2971	-9.7983
1.4	-8.9483(4)	-8.9322	0.18	-8.6411	-9.1958
2.0	-7.4486(3)	-7.4356	0.17	-7.1974	-7.6473
4.0	-4.9105(3)	-4.9019	0.18	-4.7707	-4.9959
6.0	-3.8238(2)	-3.8209	0.08	-3.7374	-3.8793
8.0	-3.244(1)	-3.2430	0.03	-3.1820	-3.2846
10.0	-2.885(1)	-2.8865	-0.05	-2.8384	-2.9185

TABLE V: Total ground state energies in units of t for the Hubbard model at half filling with open boundary conditions and total $S_z = 0$. The DMRG results used $m=1600$ renormalized states. The Jastrow factors (correlators) employed were 3-site lines for the 1D lattices and 4-site squares for the 4x5 lattice. See Sec. III C for details. Here NS, VNS, and %D have the same meaning as in Table I.

$U/t = 2$							
Lattice	VMC	NS	%D	VNS	%D	RHF	DMRG
1x14	-11.240(1)	-11.241 776	-0.02	-11.236(1)	0.04	-10.133 544	-11.279 897
1x18	-14.591(1)	-14.592 961	-0.01	-14.587(1)	0.03	-13.219 131	-14.653 987
1x22	-17.947(2)	-17.946 260	0.00	-17.938(1)	0.05	-16.307 287	-18.029 379
4x5	-19.917(1)	-19.920 320	-0.02	-19.915(1)	0.01	-18.800 678	-20.127 521

$U/t = 4$							
Lattice	VMC	NS	%D	VNS	%D	RHF	DMRG
1x14	-7.556(1)	-7.631 100	-0.99	-7.501(1)	0.73	-3.133 544	-7.672 349
1x18	-9.770(3)	-9.842 409	-0.74	-9.695(2)	0.77	-4.219 131	-9.965 398
1x22	-11.968(4)	-12.042 344	-0.62	-11.891(3)	0.64	-5.307 287	-12.259 082
4x5	-13.350(1)	-13.384 297	-0.26	-13.316(2)	0.25	-8.800 678	-14.404 488

TABLE VI: Computational time taken for various optimizations. Times are reported in total CPU hours, defined as the wall clock time multiplied by the number of processing cores used.

Lattice	Correlators	Non-Stochastic	Variational MC
8x8 Sq. Heis.	nearest neighbor	2.8×10^{-5}	1.4×10^0
8x8 Sq. Heis.	4-site squares	1.9×10^{-4}	1.4×10^0
8x8 Sq. Heis.	5-site crosses	2.7×10^{-2}	1.7×10^0
8x8 Sq. Heis.	9-site squares	4.1×10^2	3.1×10^0
6x6 Tr. Heis.	nearest neighbor	9.6×10^{-4}	3.8×10^0
6x6 Tr. Heis.	3-site triangles	8.7×10^{-4}	2.6×10^0
6x6 Tr. Heis.	4-site rhombuses	1.3×10^0	6.1×10^0
6x6 Tr. Heis.	6-site triangles	4.0×10^1	4.1×10^0
6x6 Tr. Heis.	7-site hexagons	2.1×10^1	2.4×10^0
1x14 Hub. U/t=2	3-site lines	6.7×10^{-1}	2.3×10^0
1x18 Hub. U/t=2	3-site lines	1.5×10^0	2.5×10^0
1x22 Hub. U/t=2	3-site lines	3.7×10^0	2.8×10^0
4x5 Hub. U/t=2	4-site squares	1.2×10^3	3.8×10^0
1x14 Hub. U/t=4	3-site lines	1.1×10^0	2.0×10^0
1x18 Hub. U/t=4	3-site lines	3.1×10^0	2.1×10^0
1x22 Hub. U/t=4	3-site lines	4.9×10^0	2.4×10^0
4x5 Hub. U/t=4	4-site squares	1.2×10^3	5.6×10^0

Figure Captions

FIG. 1: Examples of correlators on the square lattice. A: a 1-site correlator, similar to a Gutzwiller factor. B: a nearest-neighbor 2-site correlator. C: a 3-site line correlator. D: a 4-site line correlator. E: a 4-site square correlator. F: a 9-site square correlator. G: a 5-site cross correlator.

FIG. 2: Examples of correlators on the triangular lattice. A and B: the two orientations of 3-site triangle correlators. C and D: the two orientations of 6-site triangle correlators. E, F, and G: the three orientations of 4-site rhombus correlators. H: a 7-site hexagon correlator.

FIG. 3: Energy errors for the 20-site (4x5) spinless Hubbard model with 10 particles and open boundary conditions. The non-stochastic and variational MC methods used 4-site square Jastrow factors (correlators). Exact results were computed using the sparse diagonalization routine in the ALPS program³².

FIG. 4: Ground state energy errors for the 20-site (4x5) spinless Hubbard model with 9 particles and open boundary conditions. The non-stochastic and variational MC methods used 4-site square Jastrow factors (correlators). Exact results were computed using the sparse diagonalization routine in the ALPS program³².

FIG. 5: Energy errors (relative to $m=1600$ DMRG) in the 1D Hubbard model with $U/t = 4$ for line-shaped Jastrow factors of different sizes. The lattice is a 22 site chain with open boundary conditions. The reference function is the restricted Hartree Fock determinant. NS and VNS have the same meaning as in Table I.

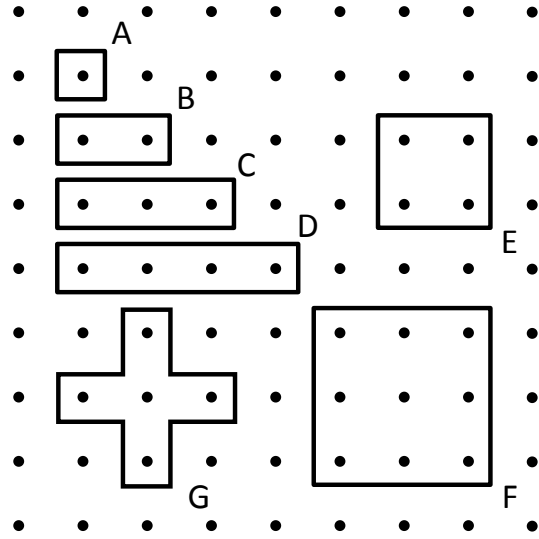


FIG. 1:

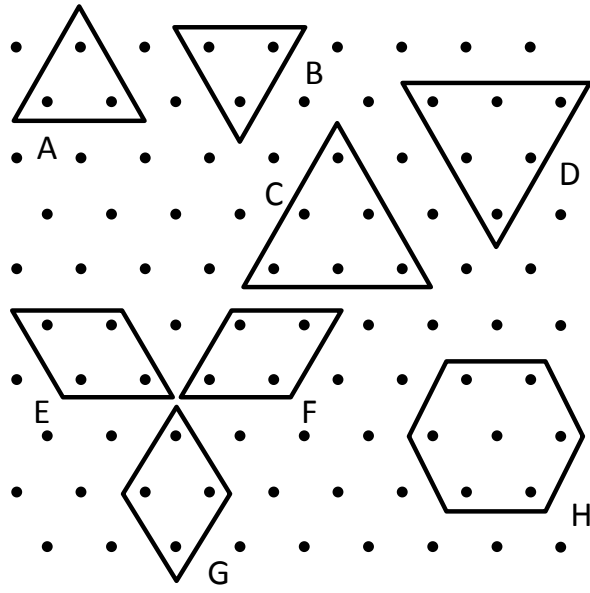


FIG. 2:

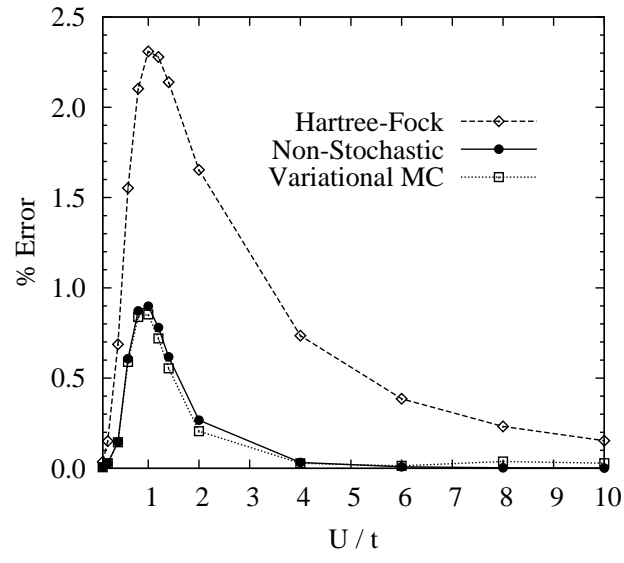


FIG. 3:

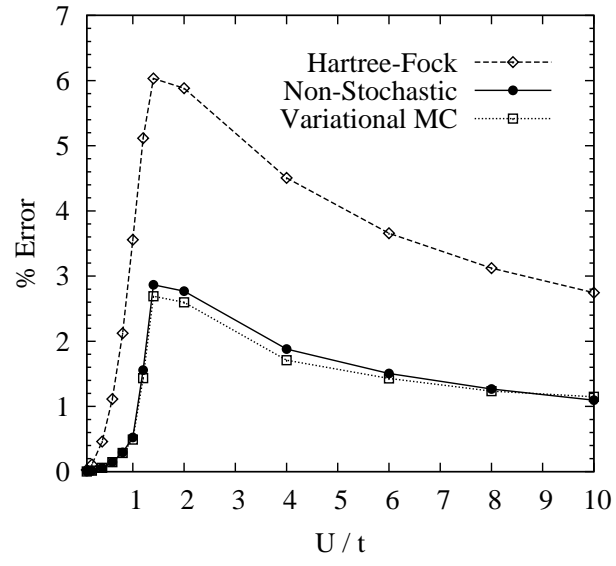


FIG. 4:

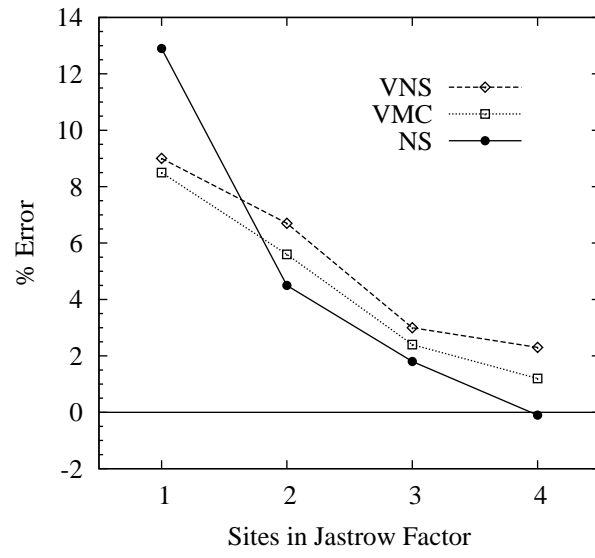


FIG. 5: