Generalized Lanczos Algorithm for Variational Quantum Monte Carlo

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We show that the standard Lanczos algorithm can be efficiently implemented statistically and self consistently improved, using the stochastic reconfiguration method, which has been recently introduced to stabilize the Monte Carlo sign problem instability. With this scheme a few Lanczos steps over a given variational wavefunction are possible even for large size as a particular case of a more general and more accurate technique that allows to obtain lower variational energies. This method has been tested extensively for a strongly correlated model like the t-J model. With the standard Lanczos technique it is possible to compute any kind of correlation functions, with no particular computational effort. By using that the variance \( \langle H^2 \rangle - \langle H \rangle^2 \) is zero for an exact eigenstate, we show that the approach to the exact solution with few Lanczos iterations is indeed possible even for \( \sim 100 \) electrons for reasonably good initial wavefunctions.

The variational stochastic reconfiguration technique presented here allows in general a many-parameter energy optimization of any computable many-body wavefunction, including for instance generic long range Jastrow factors and arbitrary site dependent orbital determinants. This scheme improves further the accuracy of the calculation, especially for long distance correlation functions.

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I. INTRODUCTION

The GFMC was introduced recently as a method to stabilize the sign problem instability in the Monte Carlo simulation, for so-called projection techniques, aiming to determine the ground state (GS) wavefunction \( \psi_0 \) of a given Hamiltonian \( H \).

In the statistical approach the electronic GS wavefunction is sampled over a set of configurations \( \{ |x> \} \), denoting spins and electron positions, and belonging to a complete basis with large or even infinite dimension. The ground state component \( \psi_0 \) of a given trial state \( \psi_G \)-henceforth assumed to be non zero on each configuration \( x \)-is filtered out by applying to it some projection operator \( G^n \) for large number \( n \) of power iterations. The matrix \( G \) maybe given by \( G = e^{-H \Delta t} \) for short imaginary time \( \Delta t \), as is the case for the conventional diffusion Monte Carlo for continuous models, or the one that will be considered in the following sections:

\[
G = (\Lambda I - H)^k_p
\]

for lattice models, where a suitably large constant shift \( \Lambda \) allows convergence to the ground state (\( \Lambda = 0 \) is used for the t-J model considered later on). The integer \( k_p \), determining the number of powers of the Hamiltonian in the Green function, may in principle larger than one, but in the following we avoid this complication and we consider \( k_p \) fixed at its minimum value: \( k_p = 1 \).

In order to perform stable simulations with large signal to noise ratio even for large \( n \) the many-body propagation \( \psi_n \rightarrow G^n |\psi_G> \) needs to be stabilized at each iteration, using an approximation that can be efficiently implemented statistically by means of the stochastic reconfiguration (SR) scheme.

The essential step in the SR is to replace the many-body state \( \psi_{n+1}^\prime (x) = G \psi_n \), obtained by applying to \( \psi_n \) the exact Green function \( G \), with the approximate state \( \psi_{n+1}^\prime (x) \), determined by the following conditions. A given set of \( p+1 \) operators \( \{ O^k \} \), not restricted to be Hermitian operator, satisfy the following equalities:

\[
\langle \psi_G | O^k | \psi_{n+1}^\prime > = \langle \psi_G | O^k | \psi_{n+1} > \quad \text{for } k = 0, \cdots, p
\]

where \( O^0 = 0 \) being the identity here for simpler and more compact notations, \( \psi_{n+1}^\prime = r_x \psi^f (x) \), \( \psi^f \) being a reference state known exactly (e.g. the standard variational approach) or statistically (e.g. the fixed node approximate state) on each configuration \( x \) and

\[
r_x = \sum_{k=0}^{p} \alpha_k O^k_x
\]

and the constants \( \alpha_k \) are determined by the conditions

\[
\alpha_i = \sum_k s_{i,k}^{-1} \langle \psi_G | O^k | \psi_{n+1} >
\]

where the covariance matrix is given by

\[
s_{i,k} = \sum_x \psi_G (x) \psi_i^f (x) O^i_x O^k_x.
\]

In this way the SR can be considered a projection \( P_{SR} \) of the exactly propagated wavefunction \( \psi_{n+1} = G \psi_n \) onto a subspace spanned by the states \( |\psi_f^k > \), defined by \( \langle x | \psi_f^k > = \langle O^k | \psi_f^k (x) \rangle \), for \( k = 0, \cdots, p \). Notice also that only when \( \psi^f = \psi_G \), \( \psi_f^k = (O^k | \psi_G > \), namely \( \psi_f^k \)
is obtained by applying the operator \((O^k)^\dagger\) to the state \(\psi_G\).

Solving the linear system determined by the SR conditions (1) we obtain a close expression for the linear operator \(P_{SR}\), which explicitly depends on the state \(\psi_G\) and the reference state \(\psi^f\):

\[
P_{SR} = \sum_{i,j} s_{ij}^{-1} |\psi^f_j \rangle \langle \psi_G|O^j
\]  

(7)

The operator \(P_{SR}\) is not a true projection operator. Though it satisfies the simple requirement (i) \(P_{SR}^2 = P_{SR}\), (ii) \(P_{SR}^\dagger = P_{SR}\) is not generally satisfied. The way to implement statistically this "pseudo"-projection operator in the large number of walker limit, was discussed in ref. 3.

After each reconfiguration the state \(\psi_n\) is replaced by \(\psi'_n = P_{SR} \psi_n\), but also the reference state \(\psi^f\) is changed. In fact in the original formulation the reference state explicitly depends on \(n\) and is updated after each SR:

\[
\psi^f_n(x) \rightarrow \text{sgn}(\psi_G(x))|\psi^f'_n(x)|.\]  

(8)

The reason of the choice (8) is to optimize the reference state and obtain more accurate results, as explained in the forthcoming paragraphs.

With the restriction of a stable simulation the signs of the reference wavefunction have to be fixed, otherwise the average sign will drop exponentially to zero in the simulation. Therefore in Eq. (8) \(\psi^f\) has been restricted to have the same signs (or the same nodes) of the guiding wavefunction \(\psi_G\). On the other hand the amplitude of the reference wavefunction \(\psi^f\) can be considerably improved from our best variational guess \(\psi_G\), since during the exact dynamic the state \(\psi_n\) gets closer to the ground state wavefunction. The optimal choice for the amplitudes has naturally led to the definition (8).

This technique, with the choice (8), has been shown to be remarkably accurate for frustrated spin or boson systems, allowing in many test-cases to obtain essentially exact results within statistical errors. However for fermion problems the situation is much different. Though this technique allows a significant improvement in the energy and correlation function calculations, the bias remains still sizable and difficult to eliminate completely by increasing the number of correlation functions used in the SR technique. Due to the antisymmetry of the fermion many body wavefunction it appears that the nodes in this case play a much more important role.

It is instructive to consider the case of continuous models. In this case, for fermion systems, nodes have to appear in the many-body wavefunction just by antisymmetry considerations. On the other hand symmetry alone does not restrict the nodal surface (the locus where the wavefunction \(\psi(x)\) vanishes), implying that correlation effects can significantly change the nodal surface. In this case it maybe useless or irrelevant to improve the amplitudes without changing the nodes in the reference wavefunction (8).

For fermion systems, due to the above difficulty to determine a nodal surface which is weakly modified by correlation effects, it appears at the moment difficult to avoid a sizable "nodal" error in energies and correlation functions. Therefore in this case it is extremely important that any approximation is at least controlled by the variational principle. In this way an approach different from the one proposed before can be used. The first step to obtain a rigorous variational method is to consider the reference wavefunction \(\psi^f\) fixed to the variational or the fixed node state. 

**II. FIXED REFERENCE DYNAMIC**

In the GFMC propagation a large number \(M\) of walkers is used, the \(j\)th walker is characterized by two weights \(w_j, w_j^f\), acting on a configuration state \(x_j\), e.g. a state with definite electron positions and spins. The reference weights \(w^f\) sample statistically the reference state \(\psi^f(x)\) whereas the weights \(w_j\) refers to the state \(\psi_j(x)\) propagated by the exact Green function \(\psi_n = G\psi_{n-1}\). More precisely, taking into account the importance sampling transformation:

\[
<< w_j \delta_{x,x_j} >> = \psi^f_n(x)\psi_G(x)\]  

(9)

\[
<< w_j \delta_{x,x_j} >> = \psi_n(x)\psi_G(x)\]  

(10)

\[
<< w_j \delta_{x,x_j} >> = \psi_n(x)\psi_G(x)\]  

(11)

where the brackets \(<<>>\) indicate both the statistical average and the one over the number of walkers, at a given Markov iteration \(n\). The two wavefunctions \(\psi^f_n\) and \(\psi_n\) are propagated, using the statistical approach. For the first state a reference Green function \(G^f_{x',x}\) with all positive matrix elements is used, whereas the latter one is propagated by means of the exact Green function \(G\) which is related to the reference one by a simple relation:

\[
G^f_{x',x} = s_{x',x} G^f_{x',x}\]  

(12)

\[
\psi_{n+1}(x')\psi_G(x') = \sum_x G_{x',x} \psi_n(x)\psi_G(x)\]  

(13)

The reference Green function \(G^f_{x',x} = p_{x',x} b_x\) is written in terms of a stochastic matrix \(p_{x',x}\) \((p_{x',x} \geq 0\) and \(\sum_{x'} p_{x',x} = 1\) times an \(x\) dependent normalization factor \(b_x = \sum_{x'} G^f_{x',x} p_{x',x}\), so that a statistical implementation of the iteration (13) is possible. Namely given the configuration \(x_j\) of the \(j\)th walker a new configuration \(x'_{j}\) is selected statistically with probability \(p_{x',x_j}\) (notice \(\sum_{x'} p_{x',x_j} = 1\) by definition):
\[ x'_j = x' \text{ with probability } p_{x',x_j}, \] (14)

Then the reference weight:

\[ w_j^f \rightarrow b_{x_j} w_j^f \] (15)

is scaled by the normalization factor \( b_{x_j} \), whereas the weight related to the exact Green function \( G \),

\[ w_j \rightarrow s_{x'_j,x_j} b_{x_j} w_j \] (16)

is further multiplied by the \( s_{x'_j,x_j} \) matrix element.

According to the above Markov iteration, defined by Eqs. (14-16) all the walkers propagate independently each others. The reference weights \( w_j^f \) remain positive, whereas the ones \( w_j \), related to the exact propagation, accumulate many sign changes, leading, for large \( n \), to an exponential increase of the signal-to-noise ratio. This is in fact determined by the corresponding exponential drop of the average walker sign \( < s > = \sum_j w_j | \sum_i w_i | \) (the infamous "sign problem"). The stochastic reconfiguration allows to alleviate this disease, by implementing statistically the operator \( P_{SR} \) described in the previous section. In practice the weights \( w_j \) are replaced by approximate weights \( p_j \), but with much larger average sign \( < s > \). The weights \( p_j \) sample statistically \( \psi_j^f(x)G(x) \) and are determined by solving the corresponding linear system (3). This is done at a given Markov iteration by averaging Eq. (3) only over the walker samples. This means that there exists a bias due to the statistical uncertainty of the quantum averages in Eq. (3). This bias however can be controlled efficiently because for large number of walkers it vanishes as \( 1/M \). In this limit \( r_x \) in Eq. (3) depends only on the configuration \( x \) as the statistical fluctuations of the constants \( \alpha_k \) can be neglected for \( M >> p \).

Another method to control much more efficiently the statistical fluctuations of the constants \( \{ \alpha_k \} \), without using a too large number of walkers, is to perform the SR scheme only after applying, at each iteration \( n \) a large number \( L_0 \) of statistical steps defined in Eqs. (4-13). In this way the statistical averages in Eq. (3) have only small fluctuations \( \propto 1/L_0 \) that can be neglected in the limit of large bin length \( L_b \), even when a small number of walkers is used. In each bin we are considering only the iteration \( n \rightarrow n+1 \) of the power method when the parameters \( \alpha_k \) of the wavefunction \( P_{SR}\psi_n \) are known and computed in the previous iteration. Thus \( \{ w_j^f \} \) evolve statistically according to G\(^T\) (Eqs. (4-13)) and new configurations \( \{ x_j \} \) are generated for the statistical sampling of \( \psi_G(x) \psi_j^f(x) = \langle \langle w_j \delta_{x,x_j} >\rangle \), whereas, inside the bin, the weights \( \{ w_j \} \) are always initialized to \( w_j = r_{x_j} w_j^f \) i.e. with the same configurations and a simple scaling of the weights it is possible to sample the propagated state \( P_{SR}\psi_n \) in all the \( L_0 \) statistical steps. Then at each step inside the bin the exact Green function \( G \) is applied statistically (Eq. (16)) in order to sample \( \psi_{n+1} = GP_{SR}\psi_n \), which is required to calculate the RHS of the SR conditions (3). At the end of the bin new \( \alpha_k \) can be computed by solving the linear system (3). It is understood that even inside the bin a branching scheme at fixed number of walkers and with a fixed number of correcting factors can be used to improve importance sampling. Whenever the length of the bin is so large that the statistical fluctuations can be neglected, the algorithm is deterministic inside the statistical uncertainties, and becomes much more efficient compared to the original scheme, where the SR conditions where applied at each step \( (L_b = 1) \). We have found instead that the most efficient scheme is to change these constants \( \alpha_k \) only when the SR conditions (3) are not satisfied within statistical errors (e.g. they are off by more than three error bars), by increasing systematically the bin length at each iteration. This scheme allows also to eliminate the bias due to the finite number of walkers \( M \), which was rather sizable in the original formulation.

After the SR, say at the iteration \( n_0 \), in order to continue the power method iteration for \( n > n_0 \), the new approximate state \( \psi'_{n_0} = P_{SR}\psi_{n_0} \) replaces \( \psi_{n_0} \) but the reference state \( \psi_j^f \) is still arbitrary. Instead of changing the reference weights with the choice \( w_j^f = |p_j| \), (implying Eq. (3) in the large number of walker limits) it is instead possible to remain with the same reference state \( \psi_{n_0} \), without changing it in the statistical sense. This is obtained by the following simple scheme. After the SR new configurations \( x'_i = x_j(i) \) are selected among the old ones \( x_j \) according to the probability \( \Pi_j = \frac{|p_j|}{\sum_i |p_i|} \). This scheme naturally defines the random index table \( j(i) \), used to improve importance sampling-as in the branching scheme for the standard diffusion Monte Carlo-and allows to continue the simulation more efficiently with equally weighted walkers \( |w_j^f| \sim \text{Const.} \). In fact in order to sample statistically the states \( \psi_n^f \) and \( \psi_j^f \) with corresponding new weights \( w_j^f \) and \( w_i^f \):

\[
\psi_i^f(x)G(x) = \langle \langle w_i \delta_{x,x_i} >\rangle \rangle \langle \langle w_i^f \delta_{x,x_i} >\rangle \rangle
\]

\[
\psi_j^f(x)G(x) = \langle \langle w_j \delta_{x,x_j} >\rangle \rangle \langle \langle w_j^f \delta_{x,x_j} >\rangle \rangle
\]

(17)

it is enough to use the so called reweighting method, which makes the above equations exact in the statistical sense:

\[
w_i^f = \bar{w} \text{ Sgn } p_{j(i)}
\]

\[
w_i^f = \bar{w} \frac{w_i^f}{|p_{j(i)}|} = \frac{|w_i^f|}{|x_i|}
\]

(18)

(19)

where \( \bar{w} = \frac{1}{M} \sum_i |p_i| \) is a constant common to all the walker weights and Sgn \( a = \pm 1 \) represents the sign of the number \( a \). The correcting factor \( \bar{w} \) is taken into account only for a finite number \( L \) of past iterations, starting e.g. from \( n - L + 1 \), otherwise the weights of the walkers may increase or decrease exponentially leading to a divergent variance. This introduces a systematic bias that vanishes
however exponentially in $L$ and decreases as $1/M$. In practice for large number of walkers it is enough to consider only few (or even none) “correcting” factors in the statistical averages, as common practice in Green Function Monte Carlo. From the reweighting method it is also clear that the choice of the probability function $\Pi_j$ is not restricted to be proportional to $p_j$. In particular we have found more convenient to use the weights corresponding to $G\psi_n$ determined after applying Eq. (16), so that the choice $\Pi_j = \sum |w_j^n|$ further improves importance sampling, with a minor change in Eqs (15,16).

$$w_i' = \frac{P_{SR}(i)}{|w_j(i)|}$$

$$w_i'' = \frac{|w_i'|}{|r_i|}$$

with $\bar{w} = \sum |w_j|$. Using the previous scheme the reference state equilibrates necessarily to the largest right eigenstate of the reference matrix $G^f$. At equilibrium the state $\psi_{SR}$ has therefore a very well compact and clear definition. It represents the maximum right eigenstate of the matrix

$$P_{SR}(A-I-H)P_{SR}, \quad (20)$$

with given $\psi^f$ in the definition of $P_{SR}$.

The method is therefore rigorously variational provided the pseudo projector $P_{SR}$ is a true projector operator, namely for $\psi^f = \psi_G$ when $P_{SR}^\dagger = P_{SR}$, as implied by Eq. (4). In this case in fact by standard linear algebra, the maximum right eigenstate of the operator (20) is the best variational state of $H$ belonging to the subspace defined by the projector $P_{SR}$ (see Appendix A).

A. Variational energy when $P_{SR} = P_{SR}^\dagger$

In the original formulation of the SR the reference Green function was defined with a slight generalization of the fixed node Green function. The Green function proposed by Hellberg and Manusakis is instead more appropriate in this context and much more convenient from the practical point of view of reducing statistical fluctuations:

$$G^{f}_{x',x} = \frac{1}{2\pi^2} |\delta_{x',x} - \psi_G(x')H_{x',x}/\psi_G(x)| \quad (21)$$

where $z_x = \sum_{x'} |\delta_{x',x} - \psi_G(x')H_{x',x}/\psi_G(x)|$, $|a|$ meaning the absolute value of the number $a$. It is simple to show that, by applying the power method with the above Green function, convergence is reached when the maximum right eigenvector $\psi_G(x)^2$ is filtered out:

$$\sum_x G^{f}_{x',x}\psi_G(x)^2 = \psi_G(x')^2 \quad (22)$$

Thus the above Green function can be used to generate statistically configurations (see Eqs (14,15)) distributed according to $\psi_G(x)^2$ with a stochastic matrix $p_{x',x} = G^{f}_{x',x}z_{x'}/z_x$.

The advantage of using the reference Green function (21) is evident when we consider its very simple relation with the exact Green function, namely:

$$s_{x',x} = G^{f}_{x',x}/G^{f}_{x',x} = \pm z_{x'} \quad (23)$$

where the sign $\pm$ is given by the sign of the Green function matrix element $\delta_{x',x} - \psi_G(x')H_{x',x}/\psi_G(x)$, and depends of course on $x$ and $x'$. Using the fixed reference algorithm in Eq. (9) $\psi^f = \psi_G$ and the operator $P_{SR}$ represents in this special case a true projector one $P_{SR}^\dagger = P_{SR}$. Thus in this case the method is rigorously variational as pointed out in the last part of the previous section.

We notice also an important property of this method. If in the SR conditions (3) only operators defined by powers of the hamiltonian $O^k = H^k$ are used, the projector $P_{SR}$ acts on the same Krilov basis (spanned by $H^k|\psi_G > , k = 0, \ldots , p$) of the well known Lanczos algorithm. Thus $(P_{SR} G P_{SR})^m|\psi_G >$ filters out the lowest energy variational state in this Krilov basis, i.e. by definition the state obtained by applying $p$ Lanczos iterations to $\psi_G$. We recover in particular a known property of the Lanczos algorithm, valid also for the SR method: the method is exact if $p$ equals the dimension of the Hilbert space.

Due to the equivalence of the Lanczos algorithm with the SR technique it is clear why, with the latter technique, it is possible to obtain rather good approximate ground state with $p$ reasonably small. In fact the convergence of the Lanczos algorithm is at least exponential in $p\equiv k$.

We have therefore derived that the Lanczos algorithm can be implemented statistically using the SR method. This allows to perform easily two Lanczos iterations on a given variational wavefunction for fairly large size systems. Furthermore the SR method allows to put several correlation functions in the (3). Since the method is strictly variational, the variational energy has necessarily to decrease by increasing the mentioned number of correlation functions.

B. Improving the variational energy

Following, by applying a finite number of exact Green function iterations to the wavefunction $\psi_{SR}$, the corresponding quantum average,

$$E^{k}_{SR} = \frac{< \psi_{SR} | G^k \psi_{SR} >}{< \psi_{SR} | G^k | \psi_{SR} >} \quad (24)$$

remains obviously variational for any $k$.

Taking into account $2k$ statistical factors $s_{x',x}$, the above quantum averages can be statistically evaluated
with the same Markov chain for which \( E_{SR} \) (\( k = 0 \)) is computed.

The sign problem can be controlled for not too large \( k \) and systematically improved variational energies can be obtained compared to the \( k = 0 \) result. However experience has shown that it is very difficult to have significant improvement over the \( k = 0 \) result for large system size.

### III. VARIATIONAL ENERGY WHEN \( P_{SR} \neq P_{SR}^\dagger \)

We have seen that by changing the definition of the reference weight after the SR was applied \( (19) \) the method is rigorously variational. However, as we have explained in the introduction, a better choice is to continue after the SR with \( w^f = |\alpha_r'| \). The rational of this choice being that the wavefunction \( \psi^f = P_{SR} \psi \) has much better amplitudes than the variational wavefunction \( \psi_G \). This allows to improve self-consistently the reference wavefunction in order to be as close as possible to the true ground state. In this way however \( \psi^f \neq \psi_G \) and the method is no longer variational in the sense that the SR state defined by the right eigenstate with maximum modulus \( |\Lambda - E_{SR}| \) eigenvalue of the matrix:

\[
P_{SR}(\Lambda - H) P_{SR} |\psi_{SR} \rangle = (\Lambda - E_{SR}) |\psi_{SR} \rangle
\]

is no longer the lowest energy one in the basis defined by \( |\psi_k^f \rangle \) \( , k = 0, 1, \ldots, p \) and \( E_{SR} \) does not necessarily bound the ground state energy.

A compromise between the two methods, is to introduce a parameter \( r \) that interpolates smoothly the two limits. This parameter enters in the reweighting relation \( (19) \) in a very simple manner:

\[
w^f_i' = \frac{w^f_i}{|\psi^f_i|^{1-r}}
\]

Notice that, when we release the fixed reference dynamics for \( r \neq 0 \) and when for large \( n \) the constants \( \{\alpha_k\} \) converge to non zero values, the reference wavefunction \( \psi^f \) is not given by averaging the configurations with the weights \( w^f \) since the relation \( \psi_{SR} = P_{SR} \psi_n(x) = r_x \psi^f(x) \) is implied by the definition of the projector \( P_{SR} \) in Eq. (24). In fact, by using Eq. (24) and that \( < w^f_i \delta_{x,x_i} > = \psi_{SR}(x) \psi_G(x) = r_x \psi^f(x) \psi_G(x) \), it is simple to derive that:

\[
<w^f_i \delta_{x,x_i} > = |r_x|^{1-r} \text{Sgn} r_x < w^f_i \delta_{x,x_i} > = |r_x|^{1-r} \text{Sgn} r_x \psi_{SR}(x) \psi_G(x) = |r_x|^r \psi^f(x) \psi_G(x)
\]

For \( r = 0 \) the method is rigorously variational, in the sense described before. It is reasonable to expect a similar behavior for \( r \ll 1 \) when \( P_{SR}^\dagger \simeq P_{SR} \), \( r = 1 \) being the optimal choice for the amplitudes of the reference wavefunction \( \psi^f \).

For \( r \neq 0 \) we assume that the infinite number of walkers or large bin \( L_b \) is taken so that the parameters \( \alpha_k \) in the definition of \( r_x \) \( (3) \) can be considered constants for large \( n \). In this case, if we take into account the reweighting \( (26) \), the reference wavefunction \( \psi^f \) is obtained as the right eigenvector \( \psi_R(x) = < w^f_i \delta_{x,x_i} > \) with maximum eigenvalue of the renormalized reference Green function \( G^f \):

\[
G^f_{x,x_i} = |r_x|^r G^f_{x,x_i}
\]

namely as \( \psi(x) = |r_x|^{-r} \psi_R(x)/\psi_G(x) \)

Then the SR state \( \psi_{SR}(x) = r_x \psi^f(x) \) is simply given in terms of this right eigenvector:

\[
\psi_{SR}(x) = R_x \psi_R(x)
\]

with \( R_x = |r_x|^{1-r} / \psi_G(x) \text{Sgn} r_x \)

Thus even when \( r \neq 0 \) the SR state can be uniquely determined. It is also clear that, since \( r_x \) is not necessarily positive or negative, the nodes can be changed and improved with respect to the nodes of the initial guess \( \psi_G \), both for \( r = 0 \) with the standard Lanczos algorithm and for \( r > 0 \). If the nodes of \( \psi_G \) are exact and the hamiltonian is not frustrated it is also possible to show that \( r = 1 \) and \( \Lambda \to \infty \) provide the exact result, with \( r_x \) positive definite.

**It is possible to compute correlation functions over \( \psi_{SR} \)**

As it is shown in App. [13] the answer is yes, and not only for correlation functions diagonal in the basis \( x \), as in the standard forward walking technique, but also for all the ones with off diagonal elements contained in the non-zero hamiltonian matrix elements. In particular it is possible to compute:

\[
< \psi_{SR} | H | \psi_{SR} \rangle \geq E_0
\]

i.e. the expectation value over the state defined by the SR conditions. This estimate is obviously variational and can be further improved, by applying a finite number of exact Green function powers to the right and to the \( L_2 \) of the hamiltonian, as in the power-Lanczos algorithm, with the difference that in this case Eq. (24) has to be evaluated with the "forward walking technique", as described in the App. [13]. In Fig. [3] we plot the evolution of the expectation value of the energy over the state \( \psi_{SR} \) as a function of the number of iterations \( n \), required by the forward walking to filter out from \( \psi_G \) its component over \( \psi_{SR} \), leading to a true variational energy estimate. We see that for \( r = 1 \), within the original SR technique, the energy expectation value can be much higher than the corresponding "mixed average" estimate (\( n = 0 \)).

This behavior can be understood in the following way, for \( r = 1 \) and for \( \Lambda \to \infty \) there is no way to improve the sign of the wavefunction over \( \psi_G \) because \( r_x \to 1 \) (\( G \) and \( G^f \) tend to the identity up to a constant and so the correction \( r_x \) to \( \psi^f \approx \psi \) for \( r = 1 \) has to became
unity up to $O(\frac{1}{L})$, whereas for $r = 0$ the Lanczos algorithm, which is $\Lambda$ independent, certainly modifies and improves the nodes. For fermion systems therefore it appears important to work with small $r$ because the nodes of the wavefunction play a particular important role in determining a good variational energy.

A different behavior is seen for correlation functions. For large $J/t = 1$, when a four particle bound state is likely to be formed, our Jastrow-Slater wavefunction is not appropriate enough, and the large distance behavior is not exactly reproduced (see Fig. 1) even when we apply to it a couple of Lanczos iterations, that, remarkably, provide a very accurate variational energy (see table).

That the qualitative behavior of this correlation function is different from the variational starting wavefunction, can be understood only when the algorithm with $r > 0$ or the FN (which is worse in energy) are used. Especially successful is the original technique $r = 1$, which improves by a factor of two the important long range behavior of $N(|R|)$, clearly displaying the features of a genuine bound state, by a decaying probability to have holes at larger and larger distances. For correlation functions diagonal in the chosen basis the nodes do not play any role and $r = 1$ or the FN itself, are likely to provide much better correlation functions. However from the previous argument about the impossibility to correct the nodes for $r = 1$ and $G, G^f \approx I$ we expect indeed that for large size the Green function $G$ tends to the identity, either because $\Lambda \propto L$, as required by the power method to converge, or because the gap to the first excited state decreases and a power iteration $\psi_{n+1} = G\psi_n$ is less and less effective for changing the wavefunction. Thus $r$ has to scale to zero for large size if we do not want to spoil too much the variational expectation value of the energy (see Fig. 1). It is remarkable that the gain in variational energy is larger and larger when the size is increased. Thus the $r > 0$ technique seems to overcome, at least partially, a serious limitation of the Lanczos algorithm, namely that in the thermodynamic limit the energy per site cannot be improved by a technique which is not size consistent. The gain in energy with $r > 0$ can instead be size consistent, since, as shown in the appendix (B), $r > 0$ corresponds to modify the reference Green function $G^f \rightarrow G^f$, similarly to what the Fixed node algorithm—which is size consistent for size consistent $\psi_G$—does.

\section*{IV. NUMERICAL IMPLEMENTATION}

In order to put efficiently a finite number $p$ of hamiltonian powers in the SR scheme it is by far more convenient to use an importance sampling strategy (see e.g. App.C), by using information of the previous $p - 1$ Lanczos iterations. A guiding wavefunction corresponding to the previous ($p - 1$) approximation $\psi_G(x) =<
\[
x^\{\frac{p-1}{2}\} \sum_{k=0}^{p} \alpha_k H^k |\psi_G\rangle = r_{p-1}(x)|\psi_G\rangle
\]

With this new guiding function the powers of the Hamiltonian can be put in the SR conditions by computing corresponding mixed average estimators:

\[
O^k_x = \frac{\langle \psi_G | H^k | x \rangle}{\langle \psi_G | x \rangle}
\]

for \( k = 0, \ldots, p \).

The advantage of using the SR scheme is clear even when we restrict this method only to the evaluation of the first few Lanczos iterations. In order to perform \( p \) Lanczos iterations, it is enough to compute only \( p \) Hamiltonian powers on a given configuration \( x \). In the conventional variational method it is always necessary to compute the expectation value of the Hamiltonian amounting to \( 2p + 1 \) powers of the Hamiltonian, leading to much more demanding numerical effort. It is also important to emphasize that within this technique the parameters \( \alpha_k \) defining the SR state, are given at the end of the SR simulation \( n \rightarrow \infty \). Once the \( \{\alpha_k\} \) are determined it is then convenient to compute correlation functions with fixed constants \( \{\alpha_k\} \), by performing statistical averages over a large bin \( L_b \) without applying the SR conditions (3) as discussed in Sec. (\( V \)). This method significantly improves the statistical fluctuations of the quantum averages over the variational state \( P_{SR} |\psi_G\rangle \).

**V. ENERGY OPTIMIZATION FOR A MANY PARAMETER VARIATIONAL WAVEFUNCTION**

The most important advantage of the SR technique is that many variational parameters can be handled at a little expense of solving a linear system (3) of corresponding size. The few Lanczos step technique, as we have discussed before, is determined only by few coefficients due to the difficulty for large size to compute many powers of the Hamiltonian on a given configuration \( x \), which is required for the evaluation of the corresponding mixed estimator \( O^k_x \).

Clearly the method discussed in Sec. (\( V \)) is not limited only to the Hamiltonian momenta correlation functions, but remains variational for arbitrary ones. In particular many kind of correlation functions can be thought to be a renormalization of the guiding wavefunction \( \psi_G \), allowing a powerful multi-parameter energy optimization similar to (3), where the variance was instead minimized. In the present chapter we assume for simplicity that all the correlation functions are used for the purpose of optimizing the variational wavefunction \( \psi_G \), and we restrict our very general analysis to variational wavefunctions of the Jastrow-Slater form, for a strongly correlated system such as the t-J model.

\[ A. \text{The variational wavefunction} \]

The Jastrow-Slater variational wavefunction can be generally written as:

\[
|\psi_G\rangle = \hat{J}|S\rangle.
\]

where \( |S\rangle \) is a determinant wavefunction, that can be obtained as an exact ground state of a generic one-body Hamiltonian of the bilinear form \( \hat{H}_{\text{BODY}} \simeq c^\dagger c + c^\dagger c^\dagger \) whereas the Jastrow factor

\[
\hat{J} = \exp(\sum_{i,j} v(i,j)n_in_j)\exp(\sum_{i,j} v^2(i,j)\sigma_i^\sigma_j^\dagger)
\]

introduces arbitrary Gaussian correlations between local charges \( n_i = \sum_{\sigma} c^\dagger_{i,\sigma} c_{i,\sigma} \) and local spins along the z-axis: \( \sigma_i^\sigma_j^\dagger = c^\dagger_{i,\sigma} c_{i,\uparrow} - c^\dagger_{i,\downarrow} c_{i,\downarrow} \). Both operators are defined on each configuration \( \{x\} \) of the chosen Hilbert space. The reason of the exponential form in the Jastrow wavefunction comes from size-consistency considerations, implying that for macroscopic and disconnected regions of space A and B the wavefunction factorizes \( \psi_{A,B} = \psi_A \otimes \psi_B \), this factorization being fulfilled by the exponential form.

Considering the \( t-J \) model the restriction of no doubly occupied sites can be thought of an infinitely negative \( v(i,i) = -\infty \) charge correlation, whereas restriction at fixed number \( N \) of particles in a finite size \( L \), can be thought of another singular Jastrow term \( \exp(-\infty(N_{\text{tot}} - N)^2) \) where \( N_{\text{tot}} = \sum_i n_i \) is the total charge operator. The latter two singular terms in the Jastrow factor are simply a restriction on the Hilbert space that can be very easily implemented without numerical instabilities.

We now consider how the symmetries of the finite size \( t-J \) model drastically restrict the still too large number of variational parameters in the Jastrow-Slater wavefunction. Translation invariance implies that the Jastrow potential depends only on the distance \( v(i,j) = v(|R_i - R_j|) \), whereas \( v^2 = 0 \) for a singlet wavefunction.

The singlet and translation symmetry imply also strong restrictions to the one-body Hamiltonian. Defining the Slater determinant. This Hamiltonian can be generally written:

\[
\hat{H}_S = \hat{H}_0 + (\hat{\Delta}_1 + \hat{\Delta})
\]

\[
\hat{\Delta}_1 = \sum_{(R,\vec{\tau})} \Delta(\vec{\tau}) (\hat{c}_{R,\uparrow}^\dagger \hat{c}_{R+\vec{\tau},\downarrow} + \hat{c}_{R+\vec{\tau},\uparrow}^\dagger \hat{c}_{R,\downarrow})
\]

where \( \hat{H}_0 = \sum_{k,\sigma} \epsilon_k \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\sigma} \) is the free electron tight binding nearest-neighbor Hamiltonian, \( \epsilon_k = -2t(cos k_x + cos k_y) - \mu \), \( \mu \) is the free-electron chemical potential and \( \hat{\Delta} \) creates all possible pairs at the various distances \( |\tau| \) with definite rotation-reflection symmetry (e.g. \( d_{x^2-y^2} \) implies \( \Delta(1,0) = -\Delta(0,1) \)).

For a generic Jastrow-Slater singlet state, satisfying all symmetries of the t-J model, a quite large number
of variational parameters are therefore available corresponding to \( v(|\tau|) \) and \( D(\tau) \) for all distances \(|\tau|\). Not all these parameters are independent, namely the substitution \( v(|\tau|) \rightarrow v(|\tau|) + \text{const.} \) does not change the wavefunction up to a constant, so that \( v(|\tau|) \) can be assumed to be zero at the maximum distance. Analogous dependence exists between the various parameters \( \Delta(\tilde{\tau}) \), since after projecting it at fixed number of particles, the ground state of the Slater determinant hamiltonian \( \tilde{H} \) can be written:

\[
|S> = \left( \sum_{R,\tau} f(\tilde{\tau}) A_{R,\tau} \gamma_{R,\tau,\downarrow}^\dagger + A_{R,\tau} \gamma_{R,\tau,\uparrow}^\dagger \right)^{N/2}|0> \quad (36)
\]

where \( f(\tau) \) is the pairing wavefunction simply related to \( \Delta(\tau) \) in Fourier transform:

\[
f(k) = \frac{\Delta(k)}{\epsilon_k + \sqrt{\epsilon_k^2 - \Delta_k^2}}
\]

where \( \epsilon_k \) in the above expression is not limited to nearest neighbor hopping.

Thus if we scale \( f(\tau) \rightarrow \text{const.} f(\tau) \) the many body wavefunction \( \tilde{S} \) remains unchanged, implying that the number of independent parameters is equal to \( N_{\text{shell}} - 1 \), where \( N_{\text{shell}} \) is the number of independent shells at \(|\tau| > 0\) consistent with the rotation-reflection symmetry of \( f \). Notice that, once in the determinant part of the wavefunction \( N_{\text{shell}} - 1 \) variational parameters are independently varied, it is useless to consider other terms, such as, for instance, the chemical potential \( \mu \) or next-nearest neighbor hopping in \( H_0 \); they always provide a suitable renormalization of \( f \) that can be sampled by the first \( N_{\text{shell}} - 1 \) parameters. Moreover by performing a particle-hole transformation in Eq.\((34)\) on the spin down \( \tilde{c}_{\tau,\downarrow}^\dagger \rightarrow (-1)^i \tilde{c}_{\tau,\downarrow}^\dagger \), the ground state of the Hamiltonian \( \tilde{H} \) is just a Slater-determinant with \( N = L \) particles. This is the reason why this variational wavefunction represents a generic Jastrow-Slater state, a standard variational wavefunction used in QMC. Using the particle-hole transformation, it is also possible to control exactly the spurious finite system divergences related to the nodes of the d-wave order parameter.

### B. Stochastic minimization

Among the correlation functions important to define the variational wavefunction two classes are important for guiding functions of the Jastrow-Slater form \( \tilde{S} \).

- the first class of operators renormalize the Slater determinant and have been identified by Filippi and Fahy\(\textsuperscript{[4]}\). \( O^k \) are defined by means of one body operators \( O^k_{1-\text{BODY}} \) by the following relation:

\[
O^k_x = \frac{\langle x|O^k_x|\psi_G>}{\langle x|\psi_G>} = \frac{\langle x|O^k_{1-\text{BODY}}|S>}{\langle x|S>}
\]

Thus for \( |\alpha_k| \) small, \( (1 + \sum_k \alpha_k O^k)|\psi_G> > J \times \exp(\sum_k \alpha_k O^k_{1-\text{BODY}})|S> \) which remains a Jastrow Slater wavefunction of the same form \( JS' \) with \( S' = \exp(\sum_k \alpha_k O^k_{1-\text{BODY}})|S> \). Since one body operators are bilinear (e.g. \( c^\dagger c \)) in fermion second-quantization operators ‘\( S' \) remains a Slater determinant. In the Jastrow-Slater case for the \( t-J \) model considered here the one-body operators read:

\[
O^k_{1-\text{BODY}} = \sum_{R,\tau \in \text{Shell} # k} S(\tau)(\tilde{c}_{\tau,\uparrow}^\dagger \tilde{c}_{\tau,\uparrow} + \tilde{c}_{\tau,\downarrow}^\dagger \tilde{c}_{\tau,\downarrow})
\]

where the sign \( S(\tau) = \pm 1 \) is determined by symmetry. Also the bar kinetic energy \( \bar{H}_0 \) is considered in this approach. According to the previous discussion the chemical potential \( \mu \) is fixed to the free electron one in \( H_0 \).

- the second class of correlation functions are the ones that appear in the Jastrow factor. They are the diagonal operators \( O^k \) – density-density \( \sum_R n_R n_{R+\tau} \) or spin-spin \( \sum_R \sigma_R^\uparrow \sigma_{R+\tau}^\uparrow \) in the chosen basis \( x \) of configurations with fixed spins and electron positions. Again for small \( \alpha \) they can be considered a renormalization of the Jastrow factor: \( J \rightarrow J \exp(\sum_k \alpha_k O^k) \). The multi-parameter minimization method can be summarized as follows:

- after each reconfiguration the factor \( r_x = \sum \alpha_k O^k_x \) is computed with given \( \alpha_k \), whose statistical fluctuations can be arbitrary reduced by increasing the number of walkers or the bin length \( L_b \) as described in Sec.(\( \text{II} \)). In this case of non linear optimization the bin technique is particular important because it allows to avoid, for large enough bin length \( L_b \), unphysical fluctuations of the guiding wavefunction.

After an exact Green function step a wavefunction better than \( \psi_G \) is obtained and is parametrized by the coefficient \( \alpha_k \) contained in the factor \( r_x \): In fact

\[
P_{SR}\psi_{n+1} = P_{SR}GP_{SR}\psi_n = r_x \psi_G(x)
\]

has to be by definition a variational state better than \( P_{SR}\psi_n \), which in turn is better than \( \psi_G \), since for instance we can assume \( \psi_{n=0} = \psi_G \).

- It is therefore convenient to change at each iteration \( n \) the guiding wavefunction:

\[
|\psi_G> \rightarrow \exp(\sum_{k=1}^p a_k O^k)|\psi_G>
\]

In the above equation we have introduced new scaled coefficients \( a_k = \alpha_k/C \) simply related to the
ones $\alpha_k$ defined by the SR conditions \(2\). This is obtained by recasting $r_x$ in a form that is more suitable for exponentiation:

\[
r_x = C \left[ 1 + \sum_{k=1}^{p} \alpha_k (O^k_x - \bar{O}^k) \right]
\]

where

\[
\bar{O}^k = \frac{\sum_x \psi_G(x)^2 O^k_x}{\sum_x \psi_G(x)^2} = \langle \langle O^k_x \delta x, x_j \rangle \rangle
\]

and $C = 1 + \sum_{k=1}^{p} \alpha_k \bar{O}^k$. The above exponentiation is justified, provided $\frac{\psi'_G}{\psi_G} \approx \frac{\psi'^*}{\psi^*}$. This is certainly fulfilled at equilibrium when for large $n \psi'_{n+1} = P_{SR} \psi'_{n+1} \propto P_{SR} \psi_n \propto \psi^*_G$, $\psi^*_G$ being the Jastrow-Slater wavefunction with lowest energy expectation value. In fact at equilibrium the SR conditions turn exactly to the Euler equations of minimum energy for $\psi^*_G$:

\[
\frac{\langle \psi^*_G | O^k | \psi^*_G \rangle}{\langle \psi^*_G | \psi^*_G \rangle} = \frac{\langle \psi^*_G | H | \psi^*_G \rangle}{\langle \psi^*_G | \psi^*_G \rangle} \tag{41}
\]

as implied by \(2\) for $\psi'_{n+1} = \psi^*_G$ and $\psi_{n+1} = G \psi'_n \propto G \psi^*_G$, and taking also into account that here for simplicity $O^0$ is the identity.

This implies that $\psi^*_G$ is a lowest energy wavefunction of the Jastrow-Slater form. There may be many local minima when the Euler’s equations are identically satisfied. In this case the SR represents a very useful tool for global minimization. In fact the bin length $L_b$ or the number of walkers $M$ represent at each iteration $n$ an effective inverse temperature that can be increased gradually following the well known “simulated annealing” statistical algorithm \(2\). As it is shown in Fig.(3), we apply this technique with very short bin length using a full translation invariant singlet wavefunction and using $x,y$ reflection symmetries without rotation symmetry. This amounts to 24 independent parameters for a 26 site cluster ($N_{shell} = 13$). In the plot we show the evolution of the short range BCS parameters $\Delta(1,0), \Delta(0,1)$ , when at the beginning $\psi_{n=0} = \psi_G$ was set with no Jastrow term $v = 0$ and the s-wave symmetric determinant defined by $\Delta(1,0) = \Delta(0,1) = 0.1t$, $\Delta_x = 0$ for $|\tau| > 1$. The s-wave symmetric solution is locally stable, but for short enough bin there is a finite tunneling probability to cross the barrier and stabilize the much lower energy solution with d-wave symmetry.

- In order to continue with the new guiding wavefunction \(3\) without another long equilibration, walker weights $w_j$ and $w'_j$ in Eqs.(3,10) can be reweighted as follows:

\[
w_j \rightarrow w_j \langle \psi^*_G(x_j) / \psi_G(x_j) \rangle
\]

\[
w'_j \rightarrow w'_j \langle \psi^*_G(x_j) / \psi_G(x_j) \rangle^2 \tag{42}
\]

in order that the new weights acting on the same configurations $x$ represent statistically Eqs.(3,10) with $\psi^f = \psi_G = \psi^*_G$ and Eq.(14) with the new guiding wavefunction $\psi^*_G$.

- For large $n$ the one-body operators corresponding to the Slater-determinant may become linearly dependent because $D$ may approach an eigenstate of a one body hamiltonian $\sum h_k O^k_{BODY}$, $\sum h_k O^k_{BODY} | S >= E | S >$, with suitable constants $h_k$ and $E$. Thus the covariance matrix $s_{k,k'}$ quickly become singular, leading to a numerical instability which is difficult to control statistically. A stable method to overcome this difficulty was found by Filippi and Fahy \(14\), essentially by taking out one operator (the one body kinetic energy) from the ones used in the linear system \(2\). Here we have found more convenient to solve the linear system \(2\):

\[
\sum s_{k,k'} \alpha_{k'} = \langle \psi_G | O^k G | \psi_n \rangle = f_k
\]
by diagonalizing first the symmetric matrix

\[ s_{k,k'} = \sum_j U_{k,j} \Lambda_j U_{k',j} \tag{43} \]

and taking out the lowest eigenvalue \( \Lambda_0 \geq 0 \) component of the positive definite matrix \( s \). This is equivalent to select in the SR another set of \( p-1 \) operators which are no longer singularly dependent. This is a perfectly legal operation for \( \Lambda_0 \sim 0 \), since the SR condition (2) is identically satisfied. Thus the resulting linear system is no longer affected by the above numerical instability:

\[ \Lambda_j \alpha'_j = \sum_k U_{k,j} f_k \tag{44} \]

with \( \alpha'_0 = 0 \) and

\[ \alpha_k = \sum_{j>0} U_{k',j} \alpha'_j \tag{45} \]

Finally we obtain a much more stable determination of \( \alpha_k \), which does not affect the result at the equilibrium, where \( \Lambda_0 \sim 0 \) and the correct Euler equations are satisfied. With this scheme also the optimization of the Jastrow parameters together with the Slater determinant ones is possible without too much effort.

- We have found that the generic situation for Jastrow-Slater wavefunctions is that the optimal determinant is actually the ground state of a one body hamiltonian \( H_{1-BODY} = \sum_k h_k O_{k-BODY} \), a particular linear combination of the chosen one body operators used in the SR conditions. This is in agreement with the Filippi-Fahy ansatz. Occasionally however, the optimal determinant turns out to be an excited state of a one body hamiltonian.

In Fig.4 and Fig.5 we show the full Jastrow-Slater optimization for the t-J model in the largest size cases where the exact solution is known 4 holes in 26 sites and 2 holes in 32 sites, respectively. We display the hole-hole correlation functions \( N(R) = \langle 1 - n_0 \rangle(1 - n_R) \rangle \) on the variational wavefunction with and without the Jastrow factor. We see that the improvement towards the exact solution is crucially dependent on the Jastrow density-density factor especially at long range distance. This behavior seem to be analogous to the one dimensional case where long range Jastrow-factors are enough to determine the anomalous long range behavior of correlation functions in one dimensional Luttinger liquids. The remarkable accuracy of the Jastrow-Slater wavefunctions is clearly limited (see e.g. Fig.3 to

the region \( J/t \lesssim 0.5 \) where pairs with d-wave symmetry repel each other and do not form many-particle bound-states as is the case for large \( J/t \) when phase separation occurs.

For the 32 site cluster the spin-translation symmetry has to be explicitly broken in the variational wavefunction by introducing a staggered magnetization \( H_0 \rightarrow H_0 - \Delta_{AF} \sum_R (-1)^h \sigma^z_R \) along the z axis. The best wavefunction compatible with reflection-rotation and translation with spin interchange \( (\uparrow\downarrow\downarrow\uparrow) \) can be conveniently parametrized by \( \Delta_{AF} \) and also a spin Jastrow factor is allowed within this class of wavefunctions. Even in this case, as shown in the corresponding Fig(3), the hole-hole correlations are almost exactly reproduced by the strong attractive Jastrow term at long distance. This means that in this small doping regime it is important to have a broken symmetry ground state, which suppress the d-wave BCS order parameter.

FIG. 4. Hole-hole correlations (upper panels) and Jastrow-Slater parameters (lower panels) for the optimal variational singlet wavefunctions with pairing wavefunction \( f \) with d-wave symmetry in a 26 site cluster t-J model.
FIG. 5. Same as in Fig. 4 for the 32 site cluster, with a broken symmetry Slater determinant wavefunction with $\Delta_{AF} = 0.2t, \Delta_{BCS} = 0.1t$ and $t'/t = -0.15$.

The next step is to perform few Lanczos steps over these variational wavefunctions which have been shown to be very accurate but not an exact representation of the ground state many body wavefunction. In the singlet case with no broken symmetry the energy as a function of the variance of the energy per site:

$$\frac{\langle \psi_G | (H/L)^2 | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle} - \left( \frac{\langle \psi_G | H/L | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle} \right)^2$$

is indeed smoothly related to the exact ground state energy. The reason is that for a good variational state the variance approaches zero as the energy becomes exact, by increasing the number of Lanczos iterations.

FIG. 6. Energy per site as a function of the number of Lanczos steps $p = 0$ (higher energy-variance) $p = 1$ (medium energy-variance) and $p = 2$ (lowest energy with non zero variance) starting from the optimal Jastrow-Slater wavefunction for 4 holes in the 26 site clusters and several $J/t$. Only for $J/t = 0$ the broken symmetry solution (with the spin Jastrow factor $v^z \neq 0$) is better than the best singlet wavefunction (triangles). The arrows indicate the exact energies, whereas the zero variance energies are the extrapolated results with a quadratic fit (continuous lines). For $J/t = 0.5$ we show the corresponding variational $p = 0$ energy and variance for the wavefunction without Jastrow term.

Whenever on a finite system a broken symmetry variational solution has much lower energy than the fully symmetric one, the Lanczos method is less effective to extrapolate to the exact value. This is shown for instance for the 26 sites at $J/t = 0$ Fig. (5) or in the 32 site 2 hole case Fig. (6). In the latter case we show also the energy as a function of the variance for the fully symmetric solution. We see in this case, that the approach to the exact solution for a singlet wavefunction is rather difficult but indeed possible.

On a finite system there is always a small energy gain to recover a state with definite spin. It is very difficult to obtain this residual energy with few Lanczos step iterations, since in order to average over the various directions of the order parameter many hamiltonian power iterations are required. However this residual energy should vanish in the thermodynamic limit if the symmetry is indeed spontaneously broken. Therefore we conclude that the small discrepancy between exact results and extrapolated ones in Figs. (5,6) is irrelevant within the above assumption, which is confirmed by simulations on much larger size, showing antiferromagnetic long range order at small doping and ferromagnetism for the $J = 0$ case. In any case the variance extrapolation with few Lanczos steps provide always a much more accurate estimate of the exact ground state energy compared to the lowest variational estimate.
VI. RESULTS AND DISCUSSION

The variational approach is certainly limited and "biased" by the "human" choice of the variational wavefunction, "believed" to be the correct one for the physical problem considered. In this paper we have described a variational approach that improves systematically any given variational wavefunction with a couple (and in principle more) Lanczos steps, with a reasonable computational effort. This approach is certainly limited, especially for large size, when few Lanczos iterations cannot remove the possible large bias of the initial variational guess. However for 2D fermionic system on a lattice, in the strong correlation regime, i.e. close to a Mott insulator state, it is very difficult to improve the best variational wavefunction obtained with the Lanczos scheme (see table). This result is particularly meaningful if we consider that in principle the FN technique is size consistent (lowers the energy per site of the variational guess even in the thermodynamic limit) and the LS technique with fixed number of iterations \( p \) is not. Thus, close to a Mott insulator, it is very important to change the nodes of the wavefunction -that the Lanczos technique allows- rather than improving only the amplitudes- as in the FN technique. It is worth mentioning, however, that the FN energy reported in the table is only an upper bound of the expectation value of the hamiltonian on the FN state. We do not know exactly how much this will lower the energy in favor of the FN technique, but we expect that this should be only a minor correction, especially for large sizes.

As shown in the table the variational energy can be further improved by using the \( r > 0 \) technique, which, within the formalism of the present paper, can be thought as a self-consistent improvement of the amplitudes and the nodes of the few Lanczos step variational wavefunction. For \( r = 1 \) the original SR scheme is recovered, which as seen in Fig.(3), maybe not the optimal choice from the variational point of view. As far as the variational energy is concerned the self-consistent approach \((r > 0)\) is not very effective (the improvement is between 20% and 30% on small size systems) for small system sizes but appears to be more and more important as the size is increased. Also correlation functions maybe qualitatively improved (Fig(1)) by the self-consistent approach, especially when a many-particle bound state appears ("stripes" or phase separation in this model) which is not contained at the variational level.

An important advantage of the standard variational approach \((r = 0)\) is that the error in the ground state energy and correlation functions can be estimated using that the variance of the energy per site \( \langle \psi_G | H | \psi_G \rangle \) in an exact calculation should be zero. The variance can be estimated systematically with high statistical accuracy for the first \( p \) Lanczos steps acting on the initial variational wavefunction \( \psi_G \). We show that the approach to the exact result maybe smooth, even for large system size and number of electrons, even when \( \psi_G \) is not particularly close to the exact result. Obvious exceptions exist and are shown here in Fig(5) for correlation functions, whereas the energy seems always better behaved (see Fig(3)).

We have tested this simple scheme in the 2D-Heisenberg model where an exact solution of energies and correlation functions is easily available by using standard techniques. The 2D-Heisenberg model has off-diagonal long-range order in the ground state, the order parameter

\[
m^2 = \frac{1}{L^2} \sum_{R,R'} \bar{S}_R \cdot \bar{S}_{R'} (-1)^{R-R'}
\]

being finite in the thermodynamic limit \( L \to \infty \). We start with the variational wavefunction in Eq.(3) obtained by projecting out the doubly occupied states to a wavefunction with d-wave n.n. BCS pairing correlations, but without any explicit antiferromagnetic order parameter. This wavefunction represents an accurate wavefunction for the quantum antiferromagnet as far as the energy is concerned, but certainly has not the right behavior at large distance, and maybe considered an RVB disordered variational wavefunction. After applying only two Lanczos iterations the 18 site size is almost exactly reproduced by this simple wavefunction, showing that at short distance the quantum antiferromagnetic wavefunction is
almost indistinguishable from an RVB one. As we increase the size, the variational energy calculation (see Fig.8) looses clearly accuracy, since the gap to the first excited state scales to zero and the Lanczos algorithm becomes correspondingly less effective. This loss of accuracy is however not dramatic (asymptotically it scales as \( \frac{1}{\sqrt{L}} \)), as shown by the similar quantitative agreement with the exact result obtained both with the 50 and the 98 site lattice (Fig.8).

![Fig. 8. Energy per site of the finite-size Heisenberg model. Comparison of exact results (indicated by arrows) and the approximate \( p = 0, 1, 2 \) Lanczos step iterations over the projected d-wave wavefunction. Continuous lines are quadratic fit of the data.](image)

Also remarkable is the correct trend of long range correlation functions as we increase the number of Lanczos iterations. As shown in the inset of Fig.(9) the linear extrapolation with the variance, which is valid for correlation functions averaged over the system volume (see App.D), is capable to detect almost the right long range magnetic order in the Heisenberg model. This is remarkable if we consider that the starting wavefunction \( \psi_G \) is disordered, as also shown in the same inset. We remark also that in this particular case the original SR algorithm for \( r = 1 \) and \( \Lambda \to \infty \) is exact since the nodes of the variational wavefunction are the correct ones.

![Fig. 9. Order parameter \( m = \sqrt{S(\pi, \pi)/L} \) in the finite-size Heisenberg model (\( S(\pi, \pi) \) being the spin isotropic antiferromagnetic structure factor). Comparison of exact results (indicated by arrows) and the approximate \( p = 0, 1, 2 \) Lanczos step iterations over the projected d-wave wavefunction. Continuous lines are quadratic fit of the data. Inset: finite-size scaling with the variational (BCS d-wave) wavefunction and with the variance extrapolated one.](image)

As anticipated the estimate of the variational error, by using that the variance has to approach zero in an exact calculation, is really effective in this case, and shows that, even for large size it is possible to reach very good quantitative estimates of energies and correlation functions (see[4]), even when the starting wavefunction is not particularly close to the exact one. In the Lanczos algorithm the variance becomes zero only when the lowest energy state non orthogonal to the initial wavefunction is reached. However we expect that the variance may reach very small values close to a "quasi eigenstate", implying the failure of the variance variational error estimate. In fact, in this case the energy optimization Lanczos technique is trapped in a local minimum, with no possibility of tunneling to the true global minimum energy. (see fig.10).

Clearly this is a well known problem in numerical optimization and the only possibility, when the exact solution is not known, is to check the various candidates for the ground state, and determine the one with the lowest energy. From another point of view, this property of the Lanczos algorithm maybe useful to estimate physically observable quantities, such as the condensation energy for a metal to became superconductor, which is just the macroscopic difference in energy between two thermodynamically stable states. From Fig.(10) an estimate of this condensation energy is \( 0.02 t \sim 100K \), in reasonable agreement with experiments on HTc cuprates[4], suggesting that the main features of d-wave superconductivity
can be understood with this simple model.

At the moment, the approach we have presented here has to be limited to very few Lanczos iterations for large size with the given computer resources. Nevertheless it is certainly systematic and unbiased as far as the approach to the ground state is concerned: the corrections to the initial guiding function depend only on the hamiltonian $H$ and no other biased approximation. Compared to the standard FN technique, it allows a systematic improvement of the starting variational wavefunction $\psi$, by correcting not only its amplitudes but also the nodes.

The extension of this technique to continuous models is straightforward. For the reference dynamic (given by $G$ in Eq.21) one can use the Langevin dynamic, as it is done in [14], so that it is possible to determine the lowest energy state obtained by applying to $\psi$ few Lanczos steps with ($r > 0$) or without self-consistency ($r = 0$) or by using a many parameter variational wavefunction, with a non linear optimization as described in Sec.(V).

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APPENDIX A: PROPERTIES OF THE OPERATOR $P_{SR}(\Lambda - H)P_{SR}$

In this appendix we focus on some properties of the matrix $P_{SR}(\Lambda - H)P_{SR}$: defined in Eq.(20).

- the maximum eigenvalue $\Lambda - E_{SR}$ of the Hermitian matrix $P_{SR}(\Lambda - H)P_{SR}$ is certainly smaller than the corresponding one $\Lambda - E_0$ of the exact Green function $\Lambda - H$. In fact be $\psi_{SR} = P_{SR}\psi_{SR}$ the normalized eigenstate of $P_{SR}(\Lambda - H)P_{SR}$ with eigenvalue $E_{SR}$, then $P_{SR}^\dagger = P_{SR}$ implies that $E_{SR} = <\psi_{SR}|H\psi_{SR}> = E_0, as \psi_{SR}$ can be considered a variational state of the exact hamiltonian $H$ with energy $E_{SR}$.

- Since $\psi_{SR}$ is obtained by applying $[P_{SR}(\Lambda - H)P_{SR}]^n$ to a given trial wavefunction. For $n \rightarrow \infty$ such propagated wavefunction will converge therefore to the lowest energy state in the subspace projected by $P_{SR}$. This implies clearly that $E_{SR}$ is lower or at most equal than the variational energy on the reference wavefunction: $<\psi_G|H|\psi_G>$ simply because $\psi_G$ belongs to this subspace.

- Since $\psi_G$ belongs to the subspace projected by $P_{SR}$, $<\psi_G|H|P_{SR} = <\psi_G|P_{SR}H$. Therefore the mixed average estimate-statistically much more convenient-

\[
E_{MA} = \frac{<\psi_G|H|\psi_{SR}>}{<\psi_G|\psi_{SR}>} = \frac{<\psi_G|P_{SR}H\psi_{SR}|\psi_{SR}>}{<\psi_G|P_{SR}|\psi_{SR}>} = E_{SR}
\]

, coincides with the variational bound $E_{SR}$ of the ground state energy, as $\psi_{SR}$ is an exact eigenstate of $P_{SR}H P_{SR}$ with eigenvalue $E_{SR}$.

APPENDIX B: FORWARD WALKING

In order to compute correlation functions over $\psi_{SR}$ it is necessary to use a slight generalization of the forward walking technique, generalized to non-symmetric matrix such as $[25]$. Moreover since in the meaningful SR limit of large number of walkers or bin length $L_b \rightarrow \infty$ the parameters $\alpha_k^r$ can be assumed constants in $r$, it is much more convenient to implement the forward walking technique without allowing any fluctuations of the random variables $\alpha_k$. This can be done easily by first evaluating the expectation value ratios $\alpha_k = <\alpha_k> / <\alpha_0>$ for $k = 1, \ldots, p$ with the standard SR algorithm, i.e. allowing the $\alpha_k$ fluctuations for each Markov iteration $n$. The second step is to perform a different simulation, usually much more efficient as far as the error bars are concerned, with $r$ determined by non random constants $\alpha_k$:

\[
r_x = 1 + \sum_{k=1}^{p} \alpha_k O_x^k
\]

If the $\alpha_k$ are determined accurately for $M, L_b$ large the SR conditions [3] will be automatically verified within error bars. The statistical or systematic error related to the determination of the constants $\alpha_k$ is also not much important. In fact even assuming that with the first simulation the constants $\alpha_k$ are determined with a non-negligible statistical error and an unavoidable systematic bias due to the finite number of walkers, the method that we will describe in the following will provide also in such a case a variational estimate of the energy with the chosen constants $\alpha_k$. The analogy of this method with the Lanczos method is evident also in this case. Even in the latter technique, a first run is usually implemented to determine the coefficients of the ground state $\alpha_k$ in the Krylov basis spanned by the initial wavefunction $\psi_0$ and the powers of the hamiltonian applied to it $\psi_0 = \psi_0 + \sum_{k=1, p} \alpha_k H^k |\psi_0>$ (with some more technical ingredient to work with an orthonormal basis). Then correlation functions over $\psi_0$ are
computed by recovering the ground state wavefunction in this basis using the determined coefficients $\alpha_k$.

Let us now focus on the implementation of the forward walking technique within the SR scheme at fixed constants $\alpha_k$. Since $\bar{G}^f$ in Eq. (28) is not symmetric its left eigenvector $\langle \psi_L | \bar{G}^f | \psi_L \rangle$ does not necessarily coincide with the corresponding right eigenvector $\psi_R$. Fortunately the matrix $\bar{G}^f$ can be easily written in terms of a symmetric matrix $\bar{G}^0$

$$\bar{G}^f_{x',x} = \alpha_x \bar{G}^0_{x',x}/\alpha_x$$

(B2)

with

$$\alpha_x = |\psi_G(x)||r_x|^2/\sqrt{z_x}$$

(B3)

$$\bar{G}^0_{x',x} = |r_x|^2 |r_{x'}|^2 / \sqrt{z_x z_{x'}} |\Lambda \delta_{x',x} - H_{x',x}|$$

(B4)

Therefore the right and the left eigenvectors of $\bar{G}^f$ are easily written in terms of the maximum eigenstate $\phi_0$ of the symmetric matrix $\bar{G}^0$, namely $\psi_R(x) = \alpha_x \phi_0(x)$ and $\psi_L(x) = \phi_0(x)/\alpha(x)$. Then using the definition of the SR state (29) it follows that also the left eigenvector of $\bar{G}^f$ can be written in terms of $\psi_{SR}$:

$$\psi_{SR}(x) = L x \psi_L(x)$$

(B5)

with $L_x = \psi_G(x) r_x / z_x$ (B6)

and $R_x = |r_x|^{-1} / \psi_G(x) \text{sgn} r_x$ (B7)

After applying several times the Green function $\bar{G}^f$ the walkers $w^f, x$ determine the state $\psi_R(x)$. Then it is possible to evaluate expectation values of any operator $O$ with given matrix elements $O_{x',x}$ by applying the following relation, which correspond to propagate $n$ times forward $\psi_R(x)$:

$$\frac{\langle \psi_{SR} | O | \psi_{SR} \rangle}{\langle \psi_{SR} | I | \psi_{SR} \rangle} = \lim_{n \to \infty} \frac{\sum_{x'} \bar{G}^f_{x',x}^n O_{x',x} \psi_{SR}(x)}{\sum_{x'} \bar{G}^f_{x',x}^n \psi_{SR}(x)}$$

(B8)

where the matrix elements of $O$ and the identity $I$ are replaced by the ones of the left-right transformed matrices $\bar{O}$ and $\bar{I}$ respectively. The explicit matrix elements of $\bar{O}$ and $\bar{I}$ in the RHS of the above equation are given by:

$$\bar{O}_{x',x} = L_{x'} \bar{O}_{x',x} r_x$$

(B9)

$$\bar{I}_{x',x} = L_{x'} R_x \delta_{x',x}$$

(B10)

This means that in the standard forward walking technique, instead of using the importance sampled matrix elements obtained with $L_x = \psi_G(x) = 1/R_x$ in Eq. (29), the slightly more involved ones (B9, B10) have to be considered. In fact by simple substitutions of these matrix elements into Eq. (B8), using also that $\sum_{x'} \bar{G}^f_{x',x}^n \psi_{SR}(x') = \psi_{SR}(x)/L_x$ (B3) and that $\psi_R(x) = \psi_{SR}(x)/R_x$ (29), Eq. (B8) is easily verified.

The statistical algorithm used to evaluate the ratio in Eq. (B8) is very similar to the standard "forward walking" technique for diagonal operators. The few differences are:

- also the denominator in Eq. (B8) has to be "forward" propagated for $n$ iterations, since in this case the diagonal elements of $\bar{I}$ are not trivially one (since $L_x \neq R_x^{-1}$). The error bars have to be then calculated taking into account that the numerator and the denominator are very much correlated.
- off diagonal operators can be computed without performing another simulation, provided the matrix elements of the operator $O$ are contained in the non vanishing ones of the Green function $G$ (or some power of $G$ if the operator is evaluated statistically). In particular the expectation value of the Hamiltonian and the even more accurate ones (24) can be computed altogether with a single Markov chain.
- similarly the accuracy of diagonal and off diagonal operators can be further improved by computing

$$\frac{\langle \psi_{SR} | G^G O^G | \psi_{SR} \rangle}{\langle \psi_{SR} | G^{2k} | \psi_{SR} \rangle}$$

In fact an important advantage of the SR technique is that the reference Green function $G^f_{x',x}$ is non zero for all non-zero elements of the exact Green function $G$, (whereas in the FN technique the matrix elements with negative sign are suppressed). Thus the exact sampling of the Green function $G$ can be done with the standard reweighting method, requiring only the finite multiplicative factors $s_{x',x} = G^f_{x',x}/G^0_{x',x}$ calculated for each iteration $n$ and each walker of the Markov chain. The same technique can be obviously generalized when the reference Green function $G^f$ is the fixed node one-slightly generalized to have the possibility to cross the nodes, simply replacing $G^f$ and $z_x = 1$ in the above expressions. However the statistical accuracy for the determination of the constants $\{\alpha_k\}$ is vary bad with the FN reference $G^f$, about an order of magnitude less efficient than the Eq. (21) one, without a significant improvement in variational energies. The reason of such bad behavior (or the successful one for [21]) is not clear at present.

APPENDIX C: EFFICIENT CALCULATION OF THE SINGLE LANCZOS STEP WAVEFUNCTION

In this Appendix we describe an efficient way to find the optimal LS wavefunction $|\psi_\alpha\rangle = (1+\alpha \hat{H})|\psi\rangle$, starting from a chosen variational guess $|\psi\rangle$, i.e., to calculate the value of $\alpha$ for which the energy
\[ E(\alpha) = \frac{\langle \psi_G | (1 + \alpha H) H (1 + \alpha H) | \psi_G \rangle}{\langle \psi_G | (1 + \alpha H)^2 | \psi_G \rangle} \]  

(C1)

has a minimum. A standard method is to calculate statistically the various powers of the Hamiltonian

\[ h_n = \frac{\langle \psi_G | H^n | \psi_G \rangle}{\langle \psi_G | \psi_G \rangle}, \]

(C2)

using configurations \( x \) generated by the Metropolis algorithm according to the weight \( \psi_G(x)^2 \). This method is however inefficient since much better importance sampling is obtained when configurations are instead generated according to the optimal Lanczos wavefunction \( \psi_\alpha(x) = (1 + \alpha e_\psi(x)) \psi_G(x) \), where \( e_\psi(x) = \langle \psi(x) | H | \psi(x) \rangle \) is the local energy corresponding to a generic guiding wavefunction \( \psi \), and \( \alpha^* \) minimizes the above expectation value (C2) for \( \alpha = \alpha^* \). This wavefunction \( \psi_\alpha^* \) may be much better leading to much lower variances especially for the higher momenta \( h_2 \) and \( h_3 \).

In this Appendix we describe an efficient way to find the optimal LS wavefunction \( | \psi_\alpha^* \rangle \), starting from a chosen variational guess \( | \psi_\alpha \rangle \) with energy:

\[ E(\alpha) = \frac{h_1 + 2a h_2 + \alpha^2 h_3}{1 + 2a h_1 + \alpha^2 h_2} \]  

(C3)

easily written in terms of the energy momenta \( h_n \).

In order to minimize (C3), given an arbitrary value of \( \alpha \), it is convenient first to compute the energy expectation value \( h_1 \) with the standard statistical method and then, in place of the remaining Hamiltonian higher momenta \( h_2 \) and \( h_3 \), generate statistically configurations according to \( \psi_\alpha(x)^2 \) and compute:

\[ E(\alpha) = \frac{\langle \psi_\alpha | H | \psi_\alpha \rangle}{\langle \psi_\alpha | \psi_\alpha \rangle}, \]

\[ \chi = \frac{\langle \psi_\alpha | (1 + \alpha H)^{-1} | \psi_\alpha \rangle}{\langle \psi_\alpha | \psi_\alpha \rangle}, \]

\[ E(\alpha) \]

is obtained by averaging over the chosen configurations the local energy corresponding to \( \psi_\alpha \), namely \( < e_\psi_\alpha > \) whereas \( \chi \) is obtained by averaging over the same configurations \( < (1 + \alpha e_\psi(x))^{-1} > \). Given \( \chi \) it is straightforward to compute

\[ h_2 = [(\chi^{-1} - 2)(1 + \alpha h_1) + 1]/\alpha^2 \]

and therefore given \( h_1 \) and \( h_2 \), the value of \( E(\alpha) \) implicitly defines the highest momentum \( h_3 = \frac{E(\alpha)(1 + 2a h_1 + \alpha^2 h_2) - h_2 - 2a h_2}{h_1 h_3 - h_2^2} \). Notice that the most difficult energy momentum \( h_3 \) is given by sampling an energy expectation value, which is by far statistically more accurate compared to the direct determination of \( h_3 \).

It is then possible to minimize analytically \( E(\alpha) \), yielding:

\[ \alpha^* = -\frac{(h_3 - h_1 h_2) \pm \sqrt{(h_3 - h_1 h_2)^2 - 4(h_2 - h_2^2)(h_1 h_3 - h_2^2)}}{2(h_1 h_3 - h_2^2)} \]  

(C4)

where the above sign \( \pm \) is such to minimize \( E(\alpha^*) \).

The analytic minimization of \( E(\alpha) \) (C4), given the values of \( \chi, h_1 \) and \( E(\alpha) \) itself, provides the exact value of \( \alpha^* \) in Eq. (C4) within the statistical uncertainties. They become smaller and smaller whenever \( \alpha \sim \alpha^* \). Typically two or at most three attempts are enough to reach an accurate determination of \( \alpha^* \) when the condition:

\[ \chi = \frac{1}{1 + \alpha^* E(\alpha^*)} \]  

(C5)

is exactly fulfilled. This condition is true in general only for the eigenstates of the Hamiltonian, but remains valid for the single Lanczos step wavefunction.

**APPENDIX D: VARIANCE ESTIMATE OF THE ERROR ON "BULK" CORRELATION FUNCTIONS**

In this appendix we estimate the error on correlation functions assuming that the ground state \( | \psi_0 \rangle \) is approximated with the wavefunction \( \psi_p \) distant \( \epsilon_p \) from \( | \psi_0 \rangle \). Namely, with no loss of generality we write:

\[ | \psi_0 \rangle = | \psi_p \rangle + \epsilon_p | \psi' \rangle \]  

(D1)

with \( < \psi_p | \psi_p > = < \psi' | \psi' > = 1 \), \( \psi' \), representing a normalized wavefunction orthogonal to the exact one \( < \psi_0 | \psi' > = 0 \). We restrict our analysis to thermodynamically averaged correlation functions \( O \), the ones which can be written as a bulk average of local operators \( O_R \): \( O = \frac{1}{R} \sum_R O_R \). This class of operators includes for instance the average kinetic or potential energy or the spin-spin correlation function at a given distance \( \tau \), \( O_R = S_R : S_{R+\tau} \). If we use periodic boundary conditions the expectation value of \( O_R \) on a state with given momentum does not even depend on \( R \) and the bulk average does not represents an approximation

\[ < \psi_0 | O_R | \psi_0 > = \frac{< \psi_0 | O | \psi_0 >}{< \psi_0 | \psi_0 >} = C. \]  

(D2)

We show here that the expectation value of bulk averaged operators \( O \) on the approximate state \( \psi_p \) satisfy the following relation:

\[ < \psi_p | O | \psi_p > = C + O(\epsilon_p^2, \epsilon_p/\sqrt{L}) \]  

(D3)

thus implying that for large enough size the expectation value (D3) approaches the exact correlation function \( C \) linearly with the variance. This allows to obtain a good accuracy with a good variational calculation, that is not easy to obtain if a term \( \sim \epsilon_p \) dominates.

The validity of the above statement is very simple to show under very general grounds. In fact by definition:

\[ < \psi_p | O | \psi_p > = C + 2\epsilon_p < \psi' | O | \psi_0 > + \epsilon_p^2 < \psi' | O | \psi' > \]  

(D4)
The term proportional to \( \epsilon \) in the above equation can be easily bounded by use of the Schwartz inequality:

\[
| < \psi'|O|\psi_0 > |^2 = | < \psi'|O-C|\psi_0 > |^2 \leq < \psi_0|(O-C)^2|\psi_0 >
\]

(D5)

The final term in the latter inequality can be estimated under the general assumption that correlation functions \( C(\tau) := < (O_R-C)(O_{R+\tau}-C) > \) decay sufficiently fast with distance \( |\tau| \), as a consequence of the cluster property:

\[
< \psi_0|(O-C)^2|\psi_0 > = (1+\epsilon^2) \frac{1}{L} \sum_\tau C(\tau).
\]

This concludes the proof of the statement of this appendix, provided \( \sum_\tau C(\tau) \) is finite for \( L \to \infty \).

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| $N$ | $L$ | $J/t$ | VMC | VMC+LS | VMC+FN | VMC+2 LS | VMC+LS +FN | Best SR | Best r | Exact  |
|-----|-----|-------|-----|--------|--------|----------|------------|--------|-------|--------|
| 22  | 26  | 0.3   | -0.6138(1) | -0.6332(1) | -0.6277(1) | -0.6381(1) | -0.6371(1) | -0.6387(1) | 0.375 | -0.64262 |
| 22  | 26  | 0.5   | -0.7647(1) | -0.7812(1) | -0.7759(1) | -0.7852(1) | -0.7841(1) | -0.7855(1) | 0.25  | -0.78812 |
| 22  | 26  | 1.0   | -1.1476(1) | -1.1672(1) | -1.1608(1) | -1.1719(1) | -1.1706(1) | -1.1724(1) | 0.25  | -1.17493 |
| 30  | 32  | 0.3   | -0.4543(1) | -0.4628(1) | -0.4611(1) | -0.46522(3) | -0.46524(3) | -0.4661(1) | 0.375 | -0.470175 |
| 84  | 98  | 0.4   | -0.6653(1) | -0.6807(1) | -0.6777(1) | -0.6865(1) | -0.68530(5) | -0.6879(2) | 0.1   | -0.692(1) |
| 50  | 98  | 0.4   | -0.9656(1) | -0.9832(1) | -0.98225(5) | -0.9886(1) | -0.98781(6) | -0.9901(2) | 0.1   | -0.9920(5) |

**TABLE I.** Energy per site in the t-J model for various variational methods. VMC is the standard variational method, VMC+LS is obtained by applying to it a Lanczos step, VMC+FN is the lattice fixed node approach, VMC+2 LS indicate the two Lanczos step variational wavefunction, VMC+LS+FN, is the fixed node over the VMC+LS wavefunction, and the "Best r" is $<\psi_{SR}|H|\psi_{SR}>$, computed by "forward walking" as described in App. (B), by optimizing the parameter $r$. The exact energy values for the largest size was estimated by the variance extrapolation. On the 98 sites, the FNLS computation takes 10 hour CPU time on a Pentium-II 400MHz, whereas the VMC+2LS wavefunction takes about 40 hours with $M = 500$ walkers for a statistical accuracy of $10^{-4}$ on the energy per site, the "best SR" another factor 8 more due to the forward walking. The computation of diagonal correlation functions instead takes a similar amount of time for all the methods, thus it is safer to compute them with the best variational method. Error bars are indicated in brackets.