

Wave function optimization in the variational Monte Carlo method

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An appropriate iterative scheme for the minimization of the energy, based on the variational Monte Carlo (VMC) technique, is introduced and compared with existing stochastic schemes. We test the various methods for the one-dimensional Heisenberg ring and the two-dimensional t - J model and show that, with the present scheme, very accurate and efficient calculations are possible, even for several variational parameters. Indeed, by using a very efficient statistical evaluation of the first and the second energy derivatives, it is possible to define a very rapidly converging iterative scheme that, within VMC, is much more convenient than the standard Newton method. It is also shown how to optimize simultaneously both the Jastrow and the determinantal part of the wave function.

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Since the seminal work of Gutzwiller, a large amount of progress has been achieved in the understanding of strongly correlated materials by means of correlated wave functions (WF). The fractional quantum Hall effect¹ and the theory—still controversial—of high-temperature superconductors² are two important ones among many other examples.

Most correlated WF, here indicated by $|\psi_G\rangle$, can be obtained^{3–5} by applying a two-body Jastrow factor J to a mean-field WF $|D\rangle$ described by a single determinant or a superconducting BCS state (SDBCS), so that

$$|\psi_G\rangle = J|D\rangle, \quad (1)$$

where J contains two-body density-density, and spin correlations. For accurate calculations, the inclusion of these two-body correlations in ψ_G is possible by means of the variational Monte Carlo (VMC) statistical approach.

However, the application of correlated WF to complex electronic systems,^{6–8} or, e.g., to describe correctly the metal-insulator transition,⁹ requires the use of many variational parameters. A drawback that has certainly limited the application of VMC to important physical and chemical problems with a large number of electrons.

In order to overcome the above limitations of VMC, in this paper we present a minimization scheme, that allows for the efficient optimization of the energy expectation value

$$E_\alpha = \frac{\langle \psi_\alpha | H | \psi_\alpha \rangle}{\langle \psi_\alpha | \psi_\alpha \rangle}, \quad (2)$$

where H is the model Hamiltonian considered, $\alpha = \alpha_1, \alpha_2, \dots, \alpha_p$ is a set of p variational parameters appearing in the WF $\psi_\alpha(x) = \langle x | \psi_\alpha \rangle$, where $|x\rangle$ denotes a configuration with defined electron spins and positions. Henceforth the symbol $\langle \rangle$ indicates the quantum expectation value over the state ψ_α , so that $E_\alpha = \langle H \rangle$. Within the Newton method (NM), in order to improve the variational parameters, $E_{\alpha+\gamma}$ is expanded quadratically in γ and minimized, then the parameters are changed $\alpha' = \alpha + \gamma$, and the iteration repeated until γ is negligible. In the following we describe an iterative technique that is based on a similar strategy, and, which, within

VMC, performs much better than standard NM.

At each iteration and for each variational parameter α_k we define¹⁰ an operator O_k , diagonal in the configuration basis, with diagonal elements

$$O_k(x) = \frac{\partial_{\alpha_k} \psi_\alpha(x)}{\psi_\alpha(x)}. \quad (3)$$

In order to simplify the derivation we assume that these operators O_k appear in the WF in the simple exponential form $\exp[\sum_k \alpha_k (O_k - \langle O_k \rangle)]$. This is certainly the case for the Jastrow factor J , where the operators O_k are just density-density or spin-spin correlations. Here for convenience we have subtracted from each O_k the corresponding average value $\langle O_k \rangle$, which provides an irrelevant multiplicative constant in the WF. For the variational parameters corresponding to the uncorrelated part $|D\rangle$, this exponential form is not exactly fulfilled, but is valid only for small changes of the variational parameters $|\psi_{\alpha+\gamma}\rangle \propto \exp[\sum_k \gamma_k (O_k - \langle O_k \rangle)] |\psi_\alpha\rangle$, namely within linear order in γ . In such a case, this expression does not provide the exact second derivative of the WF with respect to γ . Although this information is in principle required for the NM, we will show that the accurate determination of these terms is not really important within VMC, because the standard NM is rather inefficient even when these second WF derivatives are computed exactly. To this purpose we write $|\psi_{\alpha+\gamma}\rangle$ in a slightly more general form that depends on a further parameter β

$$|\psi_{\alpha+\gamma}\rangle \simeq \left[1 + \sum_k \gamma_k (O_k - \langle O_k \rangle) + \frac{\beta}{2} \sum_{k,k'} \gamma_k \gamma_{k'} (O_k - \langle O_k \rangle) (O_{k'} - \langle O_{k'} \rangle) \right] |\psi_\alpha\rangle. \quad (4)$$

As discussed before, this expansion is valid only within linear (quadratic) order in γ for $\beta \neq 1$ ($\beta = 1$ Jastrow case). We consider this more general form because the value of β can be used to improve the efficiency of the minimization

scheme within the VMC. On the other hand, it is clear that, as the minimum is approached, the nonlinear contribution proportional to β , as well as the higher-order ones, become negligible and irrelevant for the WF optimization.

By substituting expression (4) in Eq. (2), the energy can be systematically expanded in powers of γ_k

$$\Delta E = - \sum_k \gamma_k f_k + \frac{1}{2} \sum_{k,k'} \gamma_k \gamma_{k'} [S_h + (1 + \beta)G]^{k,k'}, \quad (5)$$

where

$$S_h^{k,k'} = \langle [O_k, [H, O_{k'}]] \rangle, \quad (6)$$

$$G^{k,k'} = 2 \langle (H - E_\alpha)(O_k - \langle O_k \rangle)(O_{k'} - \langle O_{k'} \rangle) \rangle$$

$$f_k = - \partial_{\alpha_k} E_\alpha = - 2 \langle (H - E_\alpha) O_k \rangle. \quad (7)$$

In the above equations we have used the Hermitian character of all the operators involved, implying for instance that $\langle O_k H \rangle = \langle H O_k \rangle$; f_k indicate the forces acting on the variational parameters and vanishing at the minimum energy condition, $S_h^{k,k'}$ represent the excitation matrix elements corresponding to the operators O_k , $G^{k,k'}$ take into account the remaining contributions appearing when the WF is not exact ($\langle H - E_\alpha \rangle \neq 0$), whereas the square brackets indicate the commutator. The WF parameters can be then iteratively changed $\alpha_k \rightarrow \alpha_k + \gamma_k$, by minimizing Eq. (5) whenever $S_h + (1 + \beta)G$ is positive definite. The minimum energy is obtained for

$$\gamma = B^{-1} \mathbf{f}, \quad (8)$$

with

$$B = S_h + (1 + \beta)G. \quad (9)$$

If B is not positive definite, the quadratic form (5) is not bounded from below, meaning that higher-order terms are important in the expansion (5). In this case the correction (8) may lead to a higher energy rather than to a lower energy WF. In order to overcome this difficulty, we change the matrix $B \rightarrow B + \mu S$ where S is the positive definite¹¹ overlap matrix

$$S^{k,k'} = \langle (O_k - \langle O_k \rangle)(O_{k'} - \langle O_{k'} \rangle) \rangle. \quad (10)$$

Similarly to the previous stochastic reconfiguration technique,¹⁰ we use the same matrix S in order to have a well-defined minimum for the energy ΔE in all cases. This is achieved by imposing the constraint that the linear WF change $\Delta \text{WF} = (|\psi_{\alpha+\gamma}\rangle - |\psi_\alpha\rangle)/|\psi_\alpha\rangle$, obtained with $\beta=0$ in Eq. (4), cannot be larger than a certain amount r . Hence the control parameter r is defined by means of the inequality

$$|\Delta \text{WF}|^2 \leq r^2, \quad (11)$$

where, from Eqs. (4) and (10), $|\Delta \text{WF}|^2 = \sum_{k,k'} \gamma_k \gamma_{k'} S^{k,k'}$. This constraint allows us to work always with a positive definite matrix B and, for small enough r , the energy is *certainly* lowered by changing the parameters according to (8). The constant $\mu \geq 0$ is nonzero whenever (9) is nonpositive definite

or $|\Delta \text{WF}|$ corresponding to (8) exceeds r . In these cases the constant μ is obtained as a Lagrange multiplier, namely by minimizing $\Delta E + \mu |\Delta \text{WF}|^2$, with the condition $|\Delta \text{WF}| = r$, which is simple to fulfill with standard iterative schemes. A similar control parameter was used in Ref. 6, by adding the identity matrix I scaled by $a_{\text{diag}} > 0$ to the Hessian, namely $B = S_h + 2G + a_{\text{diag}} I$, so that for $a_{\text{diag}} \rightarrow \infty$ the steepest descent is obtained, whereas within our scheme, for $\mu \rightarrow \infty$ the stochastic reconfiguration (SR) technique is recovered with $B = S/\Delta t$ and $\Delta t = 1/\mu$ small.¹⁰

As it is clear from its definition (7) the matrix G is zero when $\langle \psi_\alpha |$ coincides with the exact ground state, because in this case $\langle \psi_\alpha | (H - E_\alpha) = 0$. Therefore this matrix should be very small compared with S_h for a good variational WF. This implies that, by changing β in Eq. (9), we can obtain iterative methods converging to the minimum energy with approximately the same *small* number of iterations. As we will see in the following, for the optimization of the Jastrow (Jastrow and SDBCS) it is particularly convenient to use $\beta = -1$ ($\beta = 0$), so that $B = S_h + \mu S$ ($B = S_h + G + \mu S$), with μ determined by (11) when different from zero. Henceforth the $\beta = 1$ technique is indicated by NM, namely the standard Newton method used in Refs. 6 and 12, whereas the one defined by an appropriate choice of the parameter $\beta \neq 1$, is named SR with Hessian acceleration (SRH).

Statistical averages in VMC. In VMC the statistical averages required for each iteration are evaluated over M sampled configurations $\{x_i\}$ -named bin, obtained after a small equilibration, and distributed according to the square of the WF. We indicate the corresponding statistical averages with the symbol $\langle\langle \rangle\rangle$, e.g., $\langle\langle O_k(x) \rangle\rangle = 1/M \sum_i O_k(x_i)$, so that for large M $\langle\langle O_k(x) \rangle\rangle$ coincides with the exact quantum average $\langle O_k \rangle$, with a statistical accuracy $\propto 1/\sqrt{M}$.

After each bin we change the variational parameters according to Eq. (8), by using the appropriate matrix B discussed before. The SRH is stable for small enough r and may converge much faster than SR. With a larger bin length M , the value of r can be substantially increased, leading therefore to a much faster convergence within the SRH minimization scheme.

As also noted in Ref. 6, it is extremely important that the quantities evaluated within the statistical approach are obtained by means of fluctuations $\delta A(x) = A(x) - \langle\langle A(x) \rangle\rangle$ of suitable variables $A(x)$, that depend only on the electronic configuration x sampled with VMC. Therefore, it is useful to express the forces f_k , and the matrices S_h and S by appropriate fluctuation averages

$$f_k = - 2 \langle\langle \delta e_L(x) \delta O_k(x) \rangle\rangle \quad (12)$$

$$S_h^{k,k'} = \langle\langle \delta \partial_{\alpha_k} e_L(x) \delta O_{k'}(x) \rangle\rangle + (k \leftrightarrow k') \quad (13)$$

$$S^{k,k'} = \langle\langle \delta O_k(x) \delta O_{k'}(x) \rangle\rangle \quad (14)$$

$$G^{k,k'} = 2 \langle\langle \delta e_L(x) \delta O_k(x) \delta O_{k'}(x) \rangle\rangle, \quad (15)$$

where $e_L(x) = \langle \psi_\alpha | H | x \rangle / \langle \psi_\alpha | x \rangle$ is the so-called local energy. In order to derive Eq. (13) we insert a completeness

$\sum_x |x\rangle\langle x| = I$ in the right-hand side of Eqs. (6), and we also make use of the identity $\langle x|HO_k|\psi_\alpha\rangle = [\partial_{\alpha_k} e_L(x) + O_k(x)e_L(x)]\psi_\alpha(x)$. Then we notice that $\langle\langle\partial_{\alpha_k} e_L(x)\rangle\rangle = 0$ for $M \rightarrow \infty$,¹³ so that the fluctuations of $\partial_{\alpha_k} e_L(x)$ can conveniently appear in Eq. (13). This way to evaluate S_h is affected by much smaller statistical errors than the previous estimate¹² $\langle\langle\partial_{\alpha_k} e_L(x)O_{k'}(x)\rangle\rangle + (k \leftrightarrow k')$. For the same reason the matrix B , used in the iteration (8), is affected by the large noise present in G . Indeed, for $\beta = -1$, B does not depend on G and the corresponding statistical fluctuations are much reduced, especially for a large number of electrons N_e . In fact the operators O_k and the local energy scale with N_e , their fluctuations $\delta e_L, \delta O_k$ in (15) with $\sqrt{N_e}$, whereas the corresponding statistical averages for G are of order N_e , because they contribute to an extensive energy in (5). This implies zero signal to noise ratio ($\approx 1/\sqrt{N_e}$) in the matrix G [or similarly in S_h without using the correlation (13)] for large N_e compromising the efficiency of the VMC. On the other hand, it is clear that both the matrices S and S_h in Eqs. (13) and (14) are much better behaved, because they are obtained by averaging statistically quantities of order N_e , that have a mean value of the same order.

Unfortunately, for the optimization of $|D\rangle$, uncontrolled divergences in the evaluation of $S_h^{k,k'}$ appear when both indexes k and k' correspond to the SDBCS parameters. This is due to the zeros of $\langle x|D\rangle$, implying that $\partial_{\alpha_k} e_L(x) \approx -O_k(x)e_L(x)$ and $O_{k'}(x)$ wildly fluctuate in Eq. (13) because they can both diverge for $\psi_\alpha(x) \rightarrow 0$. The way to overcome this difficulty is to use $\beta = 0$ in Eq. (9) since the most relevant divergences in S_h are exactly canceled by G just for this value of β . In principle the matrix B cannot be evaluated statistically for $\beta \neq 0$ because the statistical uncertainty remains even for $M \rightarrow \infty$, due to these large fluctuations. For $\beta = 0$ and for large number of electrons N_e , the problem of zero signal to noise ratio in B cannot be avoided for Jastrow and SDBCS optimization, but can be substantially alleviated by a good WF choice, because G has the zero variance property: $G=0$ without noise, whenever ψ_α is an exact eigenstate.

Results. We have tested the simple SR method, the presently discussed SRH one, and the recently introduced NM (Ref. 6, $\beta=1$ in our notations) on simple L -sites lattice models, the one-dimensional Heisenberg model (1DHM) and the t - J model,¹⁴ because we believe they represent useful benchmarks to compare various techniques. The Jastrow factor of the initial WF was set to zero for both models. Moreover, consecutive configurations in each bin are separated by $2 \times L$ Metropolis attempts.

For the 1DHM we use a WF containing a long-range Jastrow factor in the form $\exp(1/2 \sum_{i,j} v_{i,j}^z S_i^z S_j^z) |D\rangle$ where $|D\rangle$ is a Néel state with magnetization along the x -spin axis. Here \vec{S} are usual spin-1/2 operators and projection over zero total spin- z component is also assumed. The long-range Jastrow is essential to destroy the long-range magnetic order in 1D and obtain a sensible and accurate ansatz.¹⁵ By using all spatial symmetries of the model, we remain with $L/2 - 1$ independent parameters in the Jastrow factor.

As shown in Fig. 1, with the present SRH technique, a converged value of the nearest neighbor v^z is obtained in less

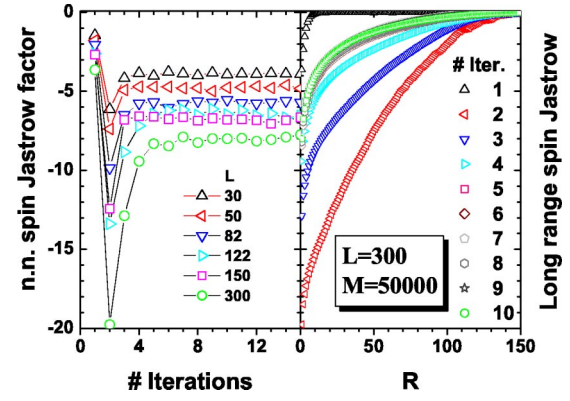


FIG. 1. (Color online) Left: convergence of the SRH technique for different sizes. Right: the same for all the 149 independent VMC parameters for the maximum size studied. For all simulations the bin length [the control parameter r defined in Eq. (11)] M was taken proportional to L^2 (L), starting from $M=500$ ($r=2$) for $L=30$.

than 10 iterations for all sizes studied [similar convergence is obtained at all distances (see right panel)], implying that the use of the matrix S_h ($\beta=-1$ has been used in this case) is very effective to accelerate the convergence to the minimum energy WF. By the SR technique, stability forces a very slow convergence: the required number of iterations increases with the system size $\propto L^2$ because the model is gapless and accurate calculations become prohibitive already for $L \approx 100$.

As shown in Fig. 2 SRH is remarkably faster than SR. After convergence, with much longer runs, SR and NM appear ≈ 50 and ≈ 10 times less efficient than SRH respectively, for obtaining the variational parameter within a given statistical error, by performing a statistical average, as discussed in Ref. 10. SR has a much larger correlation time and

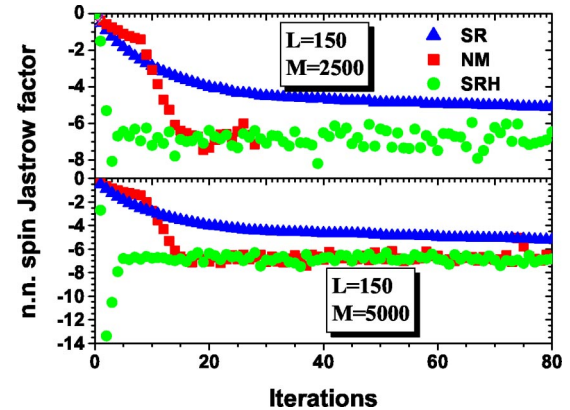


FIG. 2. (Color online) Convergence of the VMC nearest-neighbor spin Jastrow for various methods (see text). For the SR technique $\Delta t J = 0.125$. For the NM the first four iterations are with $a_{diag} = 0.02$, for the next six $a_{diag} = 0.002$, and the rest with $a_{diag} = 0$. For $M=2500$ the NM is unstable after 30 iterations due to a big fluctuation of the matrix G (see text) not used in SRH. For the SRH technique $r=5$ for $M=2500$ and $r=10$ for $M=5000$. After the third iteration $|\Delta WF| < r$ is always satisfied, even after further 1000 iterations (not shown).

NM is affected by larger fluctuations. The performances of SRH appear always optimal just for $\beta=-1$, especially for large N_e , due to the argument presented below Eq. (15). This value of β also allows us to use small bin length (see Fig. 2) and to be very efficient far away from convergence.

Optimization of $|D\rangle$. We have also tested the SRH technique in the two-dimensional (2D) t - J model at $J/t=0.4$ (Ref. 14) for optimizing the parameters contained in the $D=|H_{\text{BCS}}\rangle$ where the BCS Hamiltonian defining the H_{BCS} state has a gap function $\Delta_k=\Delta(\cos k_x-\cos k_y)$ and a dispersion band $\epsilon_k=-2(\cos k_x+\cos k_y)-4t'\cos k_x\cos k_y-\mu_0$, where μ_0 , t' , and Δ are the three variational parameters, that are optimized together with all the 40 (ten) independent ones contained in the density-density Jastrow factor $\exp(1/2\sum_{i,j}v_{i,j}n_i n_j)$ for $L=242$ ($L=50$). In this case, as discussed before, $\beta=0$ has to be used, namely $B=S_h+G$ in the iteration scheme (8). Moreover, in contrast to the Jastrow case, the condition (11) cannot be always verified with $\mu=0$ after equilibration, due to occasionally large fluctuations in the matrix B . Nevertheless, the SRH remains stable, by using a small enough value of r . In this way, these large fluctuations of B are very efficiently damped by condition (11). As shown in Fig. 3, also in this case the SRH provides a substantial reduction of the iterations required for convergence. As expected, this is accompanied also by a sizable increase of the fluctuations in the parameters especially for the chemical potential μ_0 . Indeed, though the efficiency increases with L , in favor of SRH, this improvement is not as important as in the previous case, for the optimization of the Jastrow part alone.

For the simultaneous optimization of the Jastrow and SDBCS parts of the WF, a more efficient scheme is to use the SR for the SDBCS parameters and the SRH with $\beta=-1$ for the remaining ones (hybrid method in Fig. 3). In this way, in the iteration (8), the noisy and computationally expensive (≈ 5 times more) SDBCS matrix elements $S_h^{k,k'}$ are replaced by $S^{k,k'}/\Delta t$, whereas all the other matrix elements of S_h are evaluated including also the ones coupling J

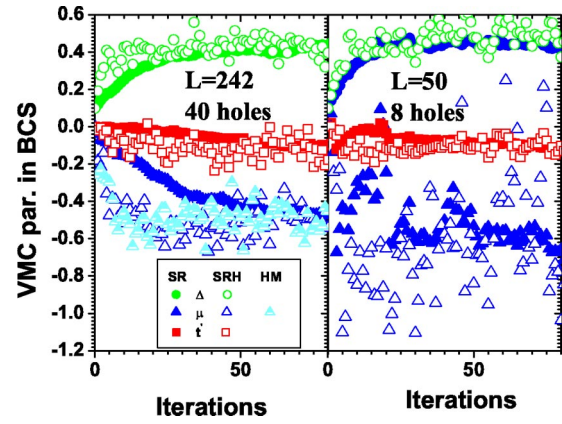


FIG. 3. (Color online) Parameters in $|D\rangle$, while optimizing the Jastrow part simultaneously for the t - J model at $J/t=0.4$ with bin $M=5000$. For SRH the control parameter is $r=0.5$ ($r=0.1$) for $L=242$ ($L=50$), for SR $J\Delta t=0.125$. The hybrid method is also shown (left) for μ_0 ($r=1$, $J\Delta t=0.3125$).

and $|D\rangle$. For these matrix elements an estimator different from the symmetric one (13) is used for S_h : $S_h^{k,k'}=S_h^{k',k}=2\langle\langle\delta\partial_{\alpha_k}e_L(x)\delta O_{k'}(x)\rangle\rangle$, involving only local energy derivatives of Jastrow parameters. After all, suitable values of r and Δt provide performances similar to SRH for the size studied, with a much cheaper computational cost per iteration and with a signal-to-noise ratio certainly stable for large N_e , as only S^h and S (and not G) are used in this case.

In conclusion, the optimization methods we have described, based on a very efficient VMC evaluation of the Hessian matrix, open the possibility to study electronic systems with correlated WF containing many variational parameters, and with an efficiency that is now comparable with the nonstatistical methods of some time ago.¹⁶

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