PHYSICAL REVIEW
LETTERS

VOLUME 82 | 24 MAY 1999 | NUMBER 21

Quantum Monte Carlo Method for Fermions, Free of Discretization Errors

S. M. A. Rombouts,* K. Heyde,† and N. Jachowicz
Universiteit Gent, Vakgroep Subatomaire en Stralingsfysica, Proeftuinstraat 86, B-9000 Gent, Belgium
(Received 20 May 1998; revised manuscript received 9 February 1999)

In this Letter we present a novel quantum Monte Carlo method for fermions, based on an exact decomposition of the Boltzmann operator $\exp(-\beta\hat{H})$. It can be seen as a synthesis of several related methods. It has the advantage that it is free of discretization errors, and applicable to general interactions, both for ground-state and finite-temperature calculations. The decomposition is based on low-rank matrices, which allows faster calculations. As an illustration, the method is applied to an analytically solvable model (pairing in a degenerate shell) and to the Hubbard model. [S0031-9007(99)09240-6]

PACS numbers: 02.70.Lq, 21.60.Ka, 71.10.Fd

Quantum Monte Carlo methods (QMC) offer an interesting way to obtain numerical results for large quantum systems [1–3]. Determinantal Monte Carlo methods that go by names as auxiliary-field [4], shell-model [5], grand-canonical [6], or projection quantum Monte Carlo [3] are based on the decomposition of the Boltzmann operator $\exp(-\beta\hat{H})$ as a sum or integral over exponentials of one-body operators. The latter are easy to handle numerically. Simple algebraic expressions exist to calculate their grand-canonical [6] or canonical trace [5,7] or their overlap between Slater determinants [3,8]. The sum or integral is then evaluated using Monte Carlo techniques, most often Markov-chain Monte Carlo techniques such as the Metropolis algorithm [9]. The basic ingredients of such a decomposition are the Suzuki-Trotter decomposition [10] to separate noncommuting parts of the Hamiltonian and the Hubbard-Stratonovich transform [11,12] to linearize the two-body part of the Hamiltonian. Both ingredients lead to systematic discretization errors in the calculations. Furthermore, for general two-body interactions these methods require many manipulations with dense matrices and hence a lot of CPU (central processing unit) time.

Several quantum Monte Carlo methods have been developed that are free from discretization errors: the Green's function QMC of Ceperley and Kalos [1], the stochastic series expansion developed by Handscomb [13] and extended by Sandvik and Kurkijärvi [14], the continuous-time loop algorithm of Beard and Wiese [15], the "worm" algorithm of Prokof'ev *et al.* [16], and the finite-temperature method for the pairing interaction developed by Cerf [17]. The latter two methods are based on the expression

$$e^{-\beta(\hat{H}_0+\hat{V})} = e^{-\beta\hat{H}_0} + \sum_{m=1}^{\infty}(-\beta)^m \int_0^{\beta} dt_m \cdots \int_0^{t_2} dt_1\, e^{-t_1\hat{H}_0}\hat{V}e^{-(t_2-t_1)\hat{H}_0}\hat{V}\cdots e^{-(t_m-t_{m-1})\hat{H}_0}\hat{V}e^{-(\beta-t_m)\hat{H}_0}. \quad (1)$$

For the determinantal QMC, no algorithm without discretization errors was available. By repeating the calculation several times, with a finer and finer mesh in imaginary time, one could make an extrapolation to the exact result. But this requires a lot of computer time.

In this Letter we present a new decomposition of the Boltzmann operator, also based on expression (1), that is free of discretization errors, but that is applicable to general interactions and moreover results in a (partially continuous) sum over exponentials of one-body operators, just like auxiliary-field quantum Monte Carlo methods. The decomposition is an exact one, so the only error in the calculations is the statistical error originating from the Monte Carlo sampling of the terms in the decomposition (apart from the round-off error due to the limited machine precision).

The trick to arrive at the decomposition of the Boltzmann operator is to replace $-\beta\hat{V}$ in expression (1) with $\mu - \beta\hat{V}$, where μ is an arbitrary, real positive parameter. Adding μ to the exponent has no influence on the properties calculated with the Boltzmann operator, and it can simply be corrected by a factor $e^{-\mu}$. Instead of expression (1) we now obtain

$$e^{-\beta\hat{H}_0+(\mu-\beta\hat{V})} = \left[1 + \sum_{m=1}^{\infty} \mu^m \int_0^1 dt_m \cdots \int_0^{t_2} dt_1 \prod_{i=1}^{m}\left(1 - \frac{\beta}{\mu}\, e^{-t_i\beta\hat{H}_0}\hat{V}e^{t_i\beta\hat{H}_0}\right)\right]e^{-\beta\hat{H}_0}. \quad (2)$$

This last expression is reminiscent of the expression for the partition function in the interaction representation derived in [18], with the difference that here the factors have the form $1 - \frac{\beta}{\mu}\hat{V}(t\beta)$ instead of $-\hat{V}(t)$ [where $\hat{V}(t)$ is the two-body Hamiltonian in the interaction representation]. It is the additional constant 1 that makes it possible to construct a decomposition into a sum of exponentials of one-body operators. To achieve this we start by constructing a decomposition for $1 - \frac{\beta}{\mu}\hat{V}$. Hereby we build on expressions derived in Ref. [19].

For the pairing Hamiltonian one has

$$\hat{V} = -G \sum_{k,k'>0} \hat{a}_{k'}^{\dagger}\hat{a}_{\bar{k}'}^{\dagger}\hat{a}_{\bar{k}}\hat{a}_k\,, \quad (3)$$

where the operator $\hat{a}_k^{\dagger}$ creates a particle in the corresponding single-particle state and with $\bar{k}$ the time-reversed state of the state k. The notation $k, k' > 0$ denotes that the summation for k and k' should run over states with angular momentum projection $j_z > 0$ only. Using lemma 1 from Ref. [19], we obtain

$$1 - \frac{\beta}{\mu}\hat{V} = \frac{1}{2\Omega^2} \sum_{k,k'>0} \sum_{s=\pm 1} \hat{\mathcal{O}}(1 + s\gamma A_{k'}^{\dagger}A_k + s\gamma A_{\bar{k}'}^{\dagger}A_{\bar{k}})\,, \quad (4)$$

with $\gamma = \Omega\sqrt{\frac{\beta G}{\mu}}$ and Ω half the number of single-particle states. A_k is the row matrix with a one on the entry corresponding to the state k, and zeros anywhere else. As defined in Ref. [19], for a square matrix Q, the operator $\hat{\mathcal{O}}(Q)$ transforms a Slater determinant Ψ_M, represented by the matrix M, into the Slater $\Psi_{M'}$, with $M' = Q\,M$. If Q is nonsingular, then $\hat{\mathcal{O}}(Q)$ is the exponential of a one-body operator. Note that this decomposition has a symmetry between the states $k > 0$ and their time-reversed states. This symmetry prevents sign problems for even particle numbers.

For the repulsive Hubbard model one can take

$$\hat{V} = U \sum_i \left(\hat{n}_{\uparrow i}\hat{n}_{\downarrow i} - \frac{\hat{n}_{\uparrow i} + \hat{n}_{\downarrow i}}{2}\right). \quad (5)$$

Then

$$1 - \frac{\beta}{\mu}\hat{V} = \frac{1}{2N_S} \sum_i [e^{\gamma(\hat{n}_{\uparrow i} - \hat{n}_{\downarrow i})} + e^{-\gamma(\hat{n}_{\uparrow i} - \hat{n}_{\downarrow i})}], \quad (6)$$

provided that $\cosh(\gamma) = 1 + \frac{U\beta N_S}{2\mu}$, with N_S the number of lattice sites and $\hat{n}_{\sigma i} = \hat{a}_{\sigma i}^{\dagger}\hat{a}_{\sigma i}$. Lemma 1 from Ref. [19] allows one to construct analogous *exact* decompositions of $1 - \frac{\beta}{\mu}\hat{V}$, based on matrices of low rank, for any fermionic interaction.

The Monte Carlo algorithm has to sample over all values of m between 0 and infinity, over all possible sets $0 \le t_1 \le \cdots \le t_m \le 1$, and at each interval over all the terms in the decomposition of $1 - \frac{\beta}{\mu}\hat{V}$. To perform this sampling numerically, a large number of intervals is taken. Let N_x be the number of intervals. To each interval i we assign a fraction τ_i of the inverse temperature, such that $\sum_{i=1}^{N_x} \tau_i = 1$, and an index I_i to indicate that part of the decomposition of $1 - \frac{\beta}{\mu}\hat{V}$ that is inserted at that interval. If no part is inserted, then $I_i = 0$. In total there are m out of N_x intervals with $I_i \neq 0$. Thus a term of order m in the decomposition (2) is represented by a configuration with m intervals for which $I_i \neq 0$. The sum of the coefficients τ_i between the jth and the $(j+1)$th insertion of $1 - \frac{\beta}{\mu}\hat{V}$ has to be equal to $t_{j+1} - t_j$. This scheme is visualized in Fig. 1.

This representation is not unique. To obtain every combination with the right weight, we have to take into account an extra weight factor $(N_x - m)!/N_x!$ for a configuration of order m. The operator corresponding to a particular configuration can then be calculated as

$$\hat{U}_{I,\tau} = \prod_{i=1}^{N_x} (e^{-\tau_i\beta\hat{H}_0}\hat{Q}_{I_i})\,, \quad (7)$$

with $\hat{Q}_j$ the jth part in the decomposition of $1 - \frac{\beta}{\mu}\hat{V}$, and $\hat{Q}_0 = 1$. From a computational point of view it is

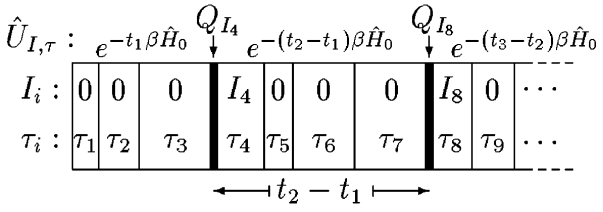

FIG. 1. A schematic way to represent the terms in the decomposition (2). The array τ_i represents the inverse-temperature intervals, the array I_i represents the parts of $1 - \frac{\beta}{\mu}\hat{V}$ that are inserted.

advantageous to work in the interaction representation, i.e.,

$$\hat{U}_{I,\tau} = \left(\prod_{i=1}^{N_x} \hat{Q}_{I_i}(t_i) \right) e^{-\beta \hat{H}_0}, \tag{8}$$

with $t_i = \sum_{k=1}^{i} \tau_k$ and $\hat{Q}_j(t)$ the jth part in the decomposition of $1 - \frac{\beta}{\mu}\hat{V}(t\beta)$. This decomposition is obtained by multiplying the row matrices used in the decomposition of $1 - \frac{\beta}{\mu}\hat{V}$, with the matrix $e^{\pm t\beta H_0}$, where H_0 is the matrix representation of the one-body operator $\hat{H}_0$ in the single-particle space. The operator $\hat{U}_{I,\tau}$ is a product of exponentials of one-body operators and thus the exponential of a one-body operator itself. Therefore, one can easily calculate its grand-canonical [6] or canonical trace [7], or apply it to a Slater determinant. In this way, exact variants of the grand-canonical [6], shell-model [5], and projector quantum Monte Carlo method [3,4] are obtained. When applying the grand-canonical or projector variant, fast updating techniques analogous to the ones presented by White *et al.* [8] can be applied. The rank-two structure in the decomposition of the factors $1 - \frac{\beta}{\mu}\hat{V}(t\beta)$ allows one to make a quick update requiring only $8N_s^2$ flops, even for general interactions. These updates have to be performed only when $I_i \neq 0$. On average, this amounts to $\langle m \rangle_{\mathrm{MC}}$ times to update the whole configuration, where $\langle m \rangle_{\mathrm{MC}}$ is value of the order m in the decomposition (2), averaged over all Monte Carlo samples. For the canonical algorithm such a fast updating technique is not possible. There the performance can be drastically improved using *guided sampling* [20]. Instead of the canonical (N-particle) weight $w_{I,\tau} = \mu^m (N_x - m)!\, \mathrm{Tr}_N(\hat{U}_{I,\tau})/N_x!$, one uses a local approximation $\tilde{w}_{I,\tau}$ that allows fast updates. After a number of steps these updates are then accepted or rejected collectively, according to the ratio $q = \frac{\tilde{w}_{I,\tau}}{\tilde{w}'_{I,r}} \frac{w'_{I,r}}{w_{I,\tau}}$. Using a generalized Metropolis algorithm [21] that includes the factor $\mu^m \frac{(N_x - m)!}{N_x!}$ in the proposition probability, one can set up a very efficient Markov chain, with acceptance rates close to unity and with autocorrelation lengths of a few sweeps.

Because the updating procedure is the most time-consuming step of the algorithm, the required CPU time will be proportional to $\langle m \rangle_{\mathrm{MC}}$. Therefore it is important to have a good estimate of this quantity in advance. If the grand-canonical or canonical algorithm is used, and if the weight $w_{I,\tau}$ is positive for all configurations, then one can show that

$$\langle m \rangle_{\mathrm{MC}} = \mu - \beta \langle \hat{V} \rangle_\beta \,. \tag{9}$$

This shows that the CPU time is proportional to the parameter μ, but also to the thermal expectation value $\langle \hat{V} \rangle_\beta$ of the residual interaction. Though μ is an arbitrary parameter, we have experienced that a good balance between low CPU cost per sweep and fast mixing of the Markov chain is obtained by taking $\mu \simeq \beta |\langle \hat{V} \rangle_\beta|$. Note that one has to take N_x such that it is always larger than the largest value of m encountered during the Monte Carlo sampling. Apart from that, the method and the CPU time it requires is independent of N_x. Expression (9) can also be used to obtain a value for $\langle \hat{V} \rangle_\beta$ from the Monte Carlo calculation. If $w_{I,\tau}$ can become negative, then one has to take into account the sign of $w_{I,\tau}$ in expression (9). To calculate expectation values for other observables, one has to use the techniques developed for auxiliary-field quantum Monte Carlo methods, as described in Refs. [5,8,22].

To test our quantum Monte Carlo method, we have applied it to a model with pairing in a degenerate shell ($\hat{H}_0 = 0$). We took $\hat{V}$ as in expression (3), with $G = 1$ MeV. This many-body problem can be solved analytically using the seniority scheme [23]. Figure 2 shows the results for the energy and the specific heat of the model, in the canonical ensemble. They agree perfectly with the analytical results. These observables were evaluated using Eqs. (11) and (14) from Ref. [22].

To make a comparison with the determinantal quantum Monte Carlo methods based on the Suzuki-Trotter decomposition, we have performed calculations for the half-filled minimal Hubbard model [24]. Hereby we used the same code for both methods. No model-specific optimizations were used, in order to allow a fair comparison between the methods. Figure 3 shows how the Coulomb and the hopping energy converge to the exact values as the size $\Delta\beta$ of the Suzuki-Trotter slices goes to zero. Figure 4 displays the corresponding CPU time required on a Digital Alpha 433 MHz workstation. A comparable precision and a much better accuracy were obtained in significantly less time using the continuous method. Results for systems away from half filling showed a similar scaling of the systematic errors and the CPU time. There the

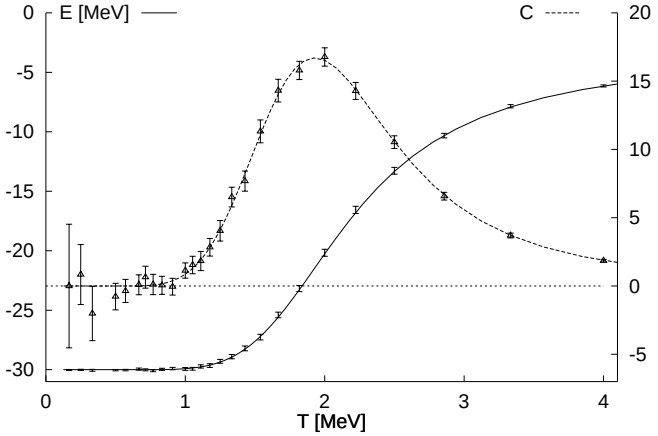

FIG. 2. Energy E and specific heat C as a function of temperature T in the canonical ensemble, for a model with pairing ($G = 1$ MeV) of 10 particles in a degenerate shell of 20 single-particle states. The curves correspond to the analytical results; the error bars indicate $2 \times 2\sigma$ intervals for the Monte Carlo results.

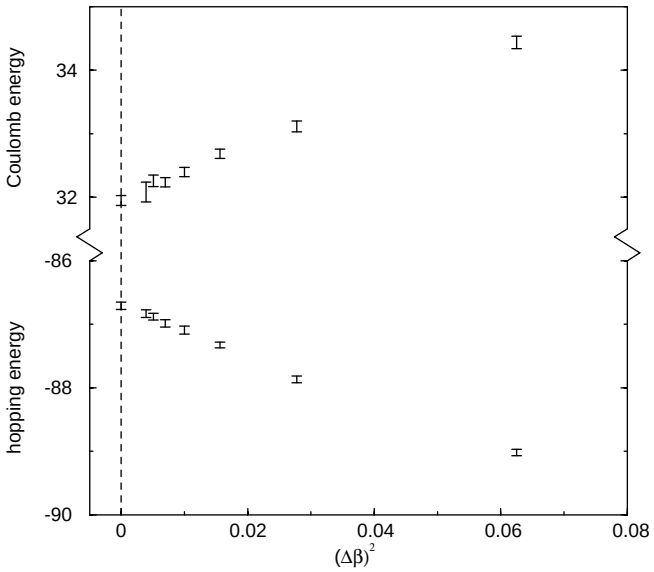

FIG. 3. Coulomb and hopping energy as a function of the inverse-temperature step $\Delta\beta$ squared, for the half-filled Hubbard model on an 8×8 lattice, with an interaction strength $U = 4|t|$, at a temperature of $T = |t|/8$ in the grand-canonical ensemble; units were chosen such that the hopping strength $|t| = 1$. The results for the continuous method are plotted at $(\Delta\beta)^2 = 0$. They were obtained with the parameter $\mu = 600$. The error bars indicate $2 \times 2\sigma$ intervals.

sign problem comes into play at low temperatures [25]. The average sign obtained was similar for both methods.

Just like other quantum Monte Carlo methods for fermions, our method is not free of sign problems at low temperatures. However, for a number of systems, a symmetry exists that guarantees good sign properties for this method. This is, among others, the case for the attractive Hubbard model, the repulsive Hubbard model at half filling, and the mean-field plus pairing model for even-even atomic nuclei, just like with the determinantal methods [22,26]. In shell-model Monte Carlo, one can exploit a specific symmetry to obtain good sign properties for the pairing + quadrupole Hamiltonian [5]. The continuous decomposition breaks this symmetry and therefore a sign problem emerges for this Hamiltonian. For other systems, one can expect the sign properties to be different from standard quantum Monte Carlo methods, because a different decomposition for the Boltzmann operator is used. This might or might not be an improvement, depending on the specific situation, but has to be studied more deeply. The idea of the constrained-path Monte Carlo method [27] can be applied here: one can put a constraint on the samples in order to obtain a good sign, thereby giving up the exactness of the method.

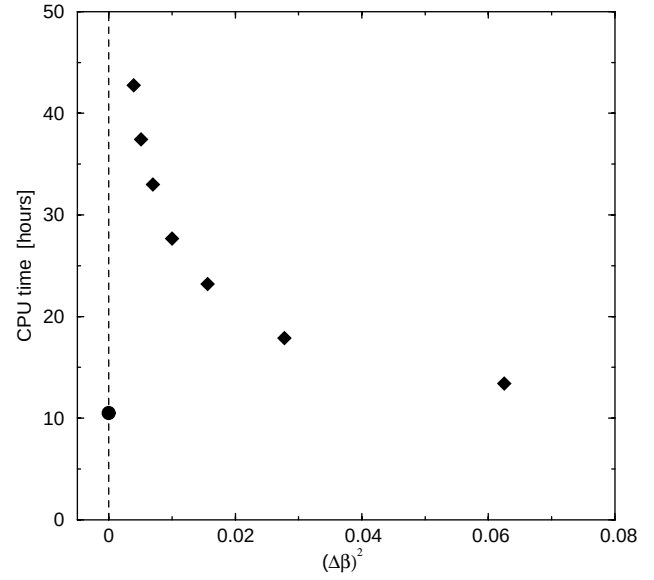

FIG. 4. Required CPU time for the corresponding data points in Fig. 3. For each set of parameters 10 000 Monte Carlo sweeps were performed.

In conclusion, we have developed a quantum Monte Carlo method for fermions based on an exact decomposition of the Boltzmann operator into a continuous sum over exponentials of one-body operators. Because of the low-rank matrices used in the decomposition, fast matrix multiplications and efficient updating procedures can be applied. The method can be applied to systems with general two-body interactions, in the grand-canonical or canonical ensemble, or with ground-state projection. It allows one to calculate thermal and ground-state expectation values for any observable. It is an exact method, apart from statistical errors.

We thank S. Zhang, J. Carlson, J. Gubernatis, A. Muramatsu, H. G. Evertz, and K. Langanke for useful discussions and comments. The work has been financially supported by the F.W.O. (Fund for Scientific Research)—Flanders and the Research Board of the University of Gent.

*Email address: Stefan.Rombouts@rug.ac.be
†Email address: Kris.Heyde@rug.ac.be

[1] D. M. Ceperley and M. H. Kalos, in *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer-Verlag, Heidelberg, 1979).
[2] D. M. Ceperley, Rev. Mod. Phys. **67**, 279 (1995).
[3] W. von der Linden, Phys. Rep. **220**, 53 (1992).
[4] G. Sugiyama and S. E. Koonin, Ann. Phys. (N.Y.) **168**, 1 (1986).
[5] S. E. Koonin, D. J. Dean, and K. Langanke, Phys. Rep. **278**, 1 (1997).
[6] R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D **24**, 2278 (1981).
[7] S. Rombouts and K. Heyde, J. Comput. Phys. **140**, 453–458 (1998).
[8] S. R. White, D. J. Scalapino, R. L. Sugar, E. Y. Loh, J. E. Gubernatis, and R. T. Scalettar, Phys. Rev. B **40**, 506 (1989).

[9] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).
[10] M. Suzuki, Phys. Lett. A **146**, 319 (1991).
[11] J. Hubbard, Phys. Rev. Lett. **3**, 77 (1959).
[12] R. D. Stratonovich, Dokl. Akad. Nauk. SSSR **115**, 1907 (1957) [Sov. Phys. Dokl. **2**, 416 (1958)].
[13] D. C. Handscomb, Proc. Cambridge Philos. Soc. **58**, 594 (1962); **60**, 115 (1964).
[14] A. W. Sandvik and J. Kurkijärvi, Phys. Rev. B **43**, 5950 (1991).
[15] B. B. Beard and U.-J. Wiese, Phys. Rev. Lett. **77**, 5130 (1996).
[16] N. V. Prokof'ev, B. V. Svistunov, and I. S. Tupitsyn, Phys. Lett. A **238**, 253 (1998).
[17] N. J. Cerf, Phys. Rev. Lett. **76**, 2420 (1996).
[18] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill Book Company, New York, 1971), p. 235.
[19] S. Rombouts, K. Heyde, and N. Jachowicz, Phys. Lett. A **242**, 271 (1998).
[20] S. Rombouts, Ph.D. thesis, University of Gent, Belgium, 1997.
[21] W. K. Hastings, Biometrika **57**, 97 (1970).
[22] S. Rombouts, K. Heyde, and N. Jachowicz, Phys. Rev. C **58**, 3295 (1998).
[23] P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer, New York, 1980), p. 221.
[24] J. Hubbard, Proc. R. Soc. London A **276**, 283 (1963); **281**, 401 (1964).
[25] E. Y. Loh, Jr., J. E. Gubernatis, R. T. Scalettar, S. R. White, D. J. Scalapino, and R. L. Sugar, Phys. Rev. B **41**, 9301 (1990).
[26] G. H. Lang, C. W. Johnson, S. E. Koonin, and W. E. Ormand, Phys. Rev. C **48**, 1518 (1993).
[27] S. Zhang, J. Carlson, and J. E. Gubernatis, Phys. Rev. Lett. **74**, 3652 (1995).