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A Novel Technique for the Simulation of Interacting Fermion Systems.

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Abstract. – A new method for the simulation of ground-state properties of interacting fermions is introduced. A trial wave function, which is assumed to be a Slater determinant, is propagated to large imaginary times. The quantum many-body propagator is represented by a coherent superposition of single-particle propagators by means of a Hubbard-Stratonovich transformation. The resulting functional integral is performed by stochastic methods based on Langevin dynamics. Numerical stability is achieved by orthonormalizing the propagating single-particle orbitals entering the Slater determinant. The problem of the positiveness of the statistical weight is addressed and solved in most cases. Illustrative examples are given for the 1D and 2D Hubbard models.

Considerable attention is presently being paid to the development of numerical methods that allow the investigation of interacting fermion systems [1]. In one way or another, all these methods face severe difficulties which are related to the antisimmetry of the fermionic wave functions.

In Green's function Monte Carlo (MC) and related methods [1, 2], these difficulties are partially circumvented by assuming a given nodal structure for the ground-state wave function. This restriction can be lifted in principle. However, the procedure for relaxing the nodal surface is computationally demanding and prone to numerical instability. This has limited the application of this more exact procedure to only a few cases.

Another class of methods is based on the MC sampling of the finite-temperature partition function $\mathcal{Z} = \mathrm{Tr}(\exp[-\beta H])$ [3-5], where $\beta = T^{-1}$ is the inverse temperature and H the Hamiltonian of the system. The ground-state properties are obtained by taking the $T \to 0$ limit. No assumption is made on the wave functions, but the $T \to 0$ limit is difficult to perform, since numerical instabilities appear in the low-T regime. These instabilities reflect the ill-conditioned nature of the determinant which is obtained once the fermionic degrees of freedom are traced out. Another severe problem is that the distribution that one has to sample by MC methods is non–positive-definite.

In this letter, we shall show that a method recently proposed by Koonin *et al.* [6] and

applied so far only to a simple boson system can be successfully extended to treat fermions. Our method does not assume any particular structure for the wave functions; the calculations are stable and give very accurate results. The problem of nonpositive definite distributions can be circumvented in most cases.

Following Koonin *et al.* [6] we introduce a projected partition function

$$Q = \langle \Psi_T | \exp[-\beta H] | \Psi_T \rangle , \tag{1}$$

where $|\Psi_T\rangle$ is a trial wave function nonorthogonal to the ground state $|\Psi_0\rangle$ and β can be thought of as an imaginary time. Since the imaginary time propagator $\exp[-\beta H]$ for $\beta \to \infty$ projects from $|\Psi_T\rangle$ its component along $|\Psi_0\rangle$ in terms of Q the ground-state energy is given by

$$E_0 \underset{\beta\to\infty}{=} -\frac{1}{\beta} \ln Q . \tag{2}$$

Expressions can be found for other ground-state properties, by differentiating eq. (2) with respect to appropriate external fields coupled to the quantities of interest.

In order to demonstrate the soundness of our procedure, we will apply our method to the 1D and 2D Hubbard model, of great current interest for its possible relevance to the physics of high-T_c superconductors [7]. The Hubbard model is described by the Hamiltonian $H = -\sum_{\langle ij\rangle,\alpha} c^\dagger_{i\alpha} c_{j\alpha} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$, where $\sum_{\langle ij\rangle}$ indicates nearest-neighbours sums, the indices run over the M lattice sites, $c^\dagger_{i\alpha}(c_{i\alpha})$ are the usual creation (annihilation) operators at site i with spin α and the two-body interaction is on site and repulsive ($U > 0$). Note, however, that our method can be extended to treat Hamiltonians with two-body interactions of fairly general range and sign.

In order to evaluate $\exp[-\beta H]|\Psi_T\rangle$ we split the imaginary-time propagator $\exp[-\beta H]$ into a product of P short-time propagators, and apply the Hubbard-Stratonovich (HS) transformation to each of them. Finally eq. (1) reads

$$Q \approx \int \mathrm{d}\sigma \exp\left[-\frac{1}{2}\sigma^2\right] \langle |\Psi_T| U_\sigma | \Psi_T \rangle , \tag{3}$$

where

$$\mathrm{d}\sigma = \prod_{j=1}^{P} \prod_{r=1}^{M} \frac{\mathrm{d}\sigma_r(j)}{\sqrt{2\pi}}, \quad \sigma^2 = \sum_{r,j} \sigma_r(j)^2 ,$$

and U_σ is the (discretized) imaginary time propagator in the time-dependent external magnetic field $\sigma_r(j)$:

$$U_\sigma \equiv U_\sigma(\beta, 0) = \exp\left[-\frac{U\beta N}{2}\right] \prod_{j=1}^{P} \exp\left[-H_0 \frac{\Delta r}{2}\right] \exp\left[-\lambda \sum_r \sigma_r(j)\, m_r\right] \exp\left[-H_0 \frac{\Delta r}{2}\right], \tag{4}$$

where H_0 is the one-body part in the Hamiltonian H, $\lambda = \sqrt{U(\beta/P)}$, $m_r = c^\dagger_{r\uparrow} c_{r\uparrow} - c^\dagger_{r\downarrow} c_{r\downarrow}$ is the magnetization operator at site r, and N is the total numer of electrons. Equation (3) becomes exact in the $P \to \infty$ limit. $U_\sigma(\beta, 0)$ can be written as a product of operators that act separately on the different spin components: $U_\sigma = U^\uparrow_\sigma U^\downarrow_\sigma$.

The most convenient form for $|\Psi_T\rangle$ is to assume that it is a Slater determinant of single-particle orbitals $|\phi^\sigma_i\rangle$ for each spin component. With this choice Q becomes $Q =$

$= \int d\sigma \exp[-\sigma^2/2] \det A_\sigma^\uparrow \det A_\sigma^\downarrow$, where A_σ^α are square matrices of components $(A_\sigma^\alpha)_{m,n} = \langle \phi_m^\alpha | U_\sigma^\alpha | \phi_n^\alpha \rangle$. These are evaluated by propagating the single-particle orbitals with the method of Fest *et al.* [8], *i.e.* by using FFT techniques and calculating potential energy propagators in real space and kinetic-energy propagators in reciprocal space, where they are diagonal in both cases. Other break-ups of the Hubbard Hamiltonians [9], or different forms of the HS transformation [4] may lead to more efficient algorithms, which are, however, difficult to extend to other Hamiltonians. Our approach is instead of more general applicability.

If we assume for the moment that $\langle \Psi_T | U_\sigma | \Psi_T \rangle$ is positive definite Q takes the form of a classical partition function: $Q = \int d\sigma \exp[-V_{\text{eff}}(\sigma)]$, where $V_{\text{eff}}(\sigma) = \frac{1}{2}\sigma^2 - \ln(\det A_\sigma^\uparrow \times \det A_\sigma^\downarrow)$. The sampling of this distribution can be done by standard means. We have preferred here to use a force biased method based on Langevin dynamics [10, 11], rather than the standard MC procedure given the highly nonlocal nature of the interaction which makes the MC update of a single degree of freedom rather costly.

In the large-β limit, a straightforward implementation of our approach undergoes numerical instabilities since the single-particle orbitals $|\phi_n^\alpha\rangle$ tend to become parallel under the action of U_σ, albeit remaining linearly independent. The numerical calculation of a determinant having all the columns nearly parallel is ill-conditioned in finite precision arithmetics. Therefore, for large enough β all the useful information is lost. This numerical instability can be successfully removed without any approximation if one takes the precaution of orthonormalizing during the propagation the single-particle orbitals. This operation is permissible because a Slater determinant of nonorthonormal orbitals can always be replaced by a determinant of orthogonalized orbitals, times a multiplicative constant. Since the orthogonalization procedure is rather costly, in practice one does not perform this operation at every imaginary time step, but at the largest interval which is compatible with the stability of the calculation.

Once the algorithm has been set up one has to find for each operator of interest, O, appropriate estimators, namely functions $E_O(\sigma)$, such that

$$\langle \Psi_0 | O | \Psi_0 \rangle \underset{\beta \to \infty}{=} Q^{-1} \int d\sigma \exp\left[-\frac{1}{2}\sigma^2\right] \det(A^\uparrow) \det(A_\downarrow) E_O(\sigma). \tag{5}$$

For instance the indicator of the density-matrix operator $c_r^\dagger c_{r'}$ is given by

$$E_{c_r^\dagger c_{r'}} = \sum_{m,n,\alpha} \phi_m^{\alpha\rangle}(r, \beta/2) A_{m,n}^{-1} \psi_n^{\alpha\langle}(r', \beta/2), \tag{6}$$

where $|\phi_m^{\alpha\rangle}(\beta/2)\rangle = U_\sigma(\beta/2, 0)|\phi_m^\alpha\rangle$, and $|\phi_m^{\alpha\langle}(\beta/2)\rangle = U_\sigma(\beta/2, \beta)|\phi_m^\alpha\rangle$.

So far we have assumed that $\langle \Psi_T | U_\sigma | \Psi_T \rangle$ is a positive definite quantity. This is in general not true. The standard procedure in this case would be to introduce the auxiliary partition function

$$Q_M = \int d\sigma \exp\left[-\frac{1}{2}\sigma^2\right] |\langle \Psi_T | U_\sigma | \Psi_T \rangle| \tag{7}$$

and to relate averages in the Q_M ensemble denoted by $\langle\ \rangle_M$ to the needed averages in the Q ensemble by

$$\langle A \rangle = \frac{\langle A \times s \rangle_M}{\langle s \rangle_M}, \tag{8}$$

where $s = \text{sign}\langle \Psi_T | U_\sigma | \Psi_T \rangle$. This method relies on the fact that $\langle s \rangle_M \neq 0$. However, very often $\langle s \rangle_M$ is very small and its variance very large. Thus estimates based on eq. (8) are subject to a large numerical uncertainty and require long simulation runs in order to converge to a reliable value. We show below that for the calculation of ground-state properties this is an unnecessarily complicated procedure.

To this end, we consider first the $\beta \to \infty$ limit of $Q/Q_M = \langle s \rangle_M$. It can be shown [12] that $\langle s \rangle_M$ is either bounded from below by $|\langle \Psi_0 | \Psi_T \rangle|^2$, or it vanishes exponentially with β for $\beta \to \infty$. In the latter case any calculation is hopelessly difficult as it would be a calculation based on eq. (8). However, if the following condition is satisfied for any β:

$$\langle s \rangle_M \geq |\langle \Psi_0 | \Psi_T \rangle|^2, \tag{9}$$

from the asymptotic behaviour of Q, it follows that $Q_M = h_M(\beta) \exp[-\beta E_0]$, where $h_M(\beta)$ is bounded for $\beta \to \infty$. Thus the ground-state energy can be obtained as: $E_0 \underset{\beta \to \infty}{=} -\frac{1}{\beta} \ln Q_M$. The consequence of this is that Q_M can replace Q in the calculation of ground-state properties. The use of Q_M, however, presents some technical difficulties since the corresponding classical potential energy is singular along the nodal surface of $\langle \Psi_T | U_\sigma | \Psi_T \rangle$ and this breaks up the integration domain into disconnected regions separated by infinite potential barriers. This difficulty can be removed and the statistical quality of the results further improved by introducing a third partition function

$$Q_N = \int \mathrm{d}\sigma \exp\left[-\frac{1}{2}\sigma^2\right] \langle \phi_T | U_\sigma^\dagger U_\sigma | \phi_T \rangle^{1/2}. \tag{10}$$

It will be shown elsewhere [12] that Q_N satisfies the following inequalities:

$$Q_M(\beta) \leq Q_N(\beta) \leq D Q_M(2\beta)^{1/2}, \tag{11}$$

where D is the (finite) dimension of the Hilbert space. If $\langle s \rangle_M \geq |\langle \Psi_0 | \Psi_T \rangle|^2$, then $Q_N(\beta) = h_N(\beta) \exp[-E_0 \beta]$ and one must have again $E_0 \underset{\beta \to \infty}{=} -\frac{1}{\beta} \ln Q_N$. Therefore, Q_N can be used to calculate ground-state properties, if for $\beta \to \infty$ $\langle s \rangle_M \neq 0$.

In order to check the above theory, we have performed calculations on 1D and 2D Hubbard models. The 1D case has been solved analytically by Lieb and Wu (LW) [13]. From their solution, we can extract ground-state energies for finite-size systems. Thus we have the possibility of a direct check of our method. In fig. 1 we display the total and kinetic energy for filling $\nu = N/M = 3/4$ as a function of U, and $M = 8$.

The comparison with the LW results for the same size system is very favourable and can be further improved by increasing the statistics as shown for the particular case $U = 8$. In 1D, we have found in all the cases explored, that an appropriate choice of $|\Psi_T\rangle$ leads to a positive definite $\langle \Psi_T | U_\sigma | \Psi_T \rangle$. We have also verified that our choice of β, P, and of the Langevin integration time step lead to errors smaller than the statistical uncertainty.

In 2D, no exact solution is available except for the 2×2 case which can be mapped onto a 4 site one-dimensional ring [14]. In the 2D half-filled case it is always possible to find trial wave functions such that $\langle \Psi_T | U_\sigma | \Psi_T \rangle \geq 0$, thus the sampling presents no sign problem. Our findings are summarized in table I. They are in excellent agreement with the 2×2 data and in line with previous numerical estimates. Away from half-filling, we have not been able to

find a trial wave function such that $\langle \Psi_T | U_\sigma | \Psi_T \rangle \geqslant 0$. We have therefore to check that we are in a favourable situation, namely that for $\beta \to \infty$, $\langle s \rangle_M$ does not vanish exponentially. This is

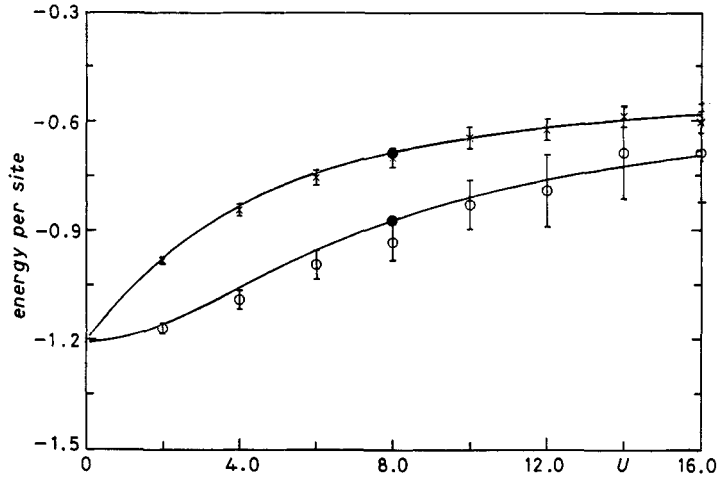

Fig. 1. – Total (upper curve) and kinetic (lower curve) energies for the 8-site 1D Hubbard model, for $\nu = 3/4$, as a function of U. The continuous line indicates the exact results by the method of Lieb and Wu. Open circles indicate simulations where averages were taken over ≈ 100 Langevin time steps. The full dots refer to a run of 2500 time steps. In this case, the error bar is smaller than the size of the dot.

TABLE I. – *Ground-state energy per site for a* 2D *square-lattice Hubbard model for different sizes and values of the interaction U. The electron density is always fixed to one electron per site. In typical simulations, β ranges from* 10 *to* 20, $P \approx 4\beta U$, *and the Langevin time step ranges from* 0.1 *to* 0.3. *Averages were taken over several thousands of configurations after suitable equilibration.*

Size	$U = 4$	$U = 8$	$U = 16$
2×2	$-1.40_5 \pm 0.06$	-1.04 ± 0.01	-0.65 ± 0.015
2×2 (*)	-1.414	-1.051	-0.6601
4×4	-0.85 ± 0.06	-0.53 ± 0.06	-0.26 ± 0.05
8×8	-0.86 ± 0.04	-0.53 ± 0.04	-0.28 ± 0.06

(*) Exact results from Lieb and Wu equations.

shown in fig. 2, where we plot $\langle s \rangle_M$ for a 4×4 system at $U = 8$, filling $\nu = 5/8$, and a Hartree-Fock trial wave function. We see that $\langle s \rangle_M$ tends to a finite limit, and we can, therefore, apply the theory developed above for obtaining estimates for the ground-state energy based on Q_N. After a linear extrapolation to $T = 0$ from values calculated for $\beta < 16$, we find: $E_0 = = -1.09 \pm 0.01$. A consistent estimate can be obtained using eq. (8). However, in this case at lower temperatures the error bars are so large that we can extrapolate only from $\beta \leqslant 4$. Thus this second estimate is subject to much larger uncertainties. For larger sizes $\langle s \rangle_M$ becomes so small that an adequate estimation is impossible. One has in these cases to rely only on Q_N. Although we have not yet been able to prove that for a generic determinantal wave function eq. (9) is satisfied, we believe that this is indeed the case. Furthermore, the internal consistency of the theory can be checked numerically in many different ways. Based on these considerations, we have been able to perform calculations on systems of size much

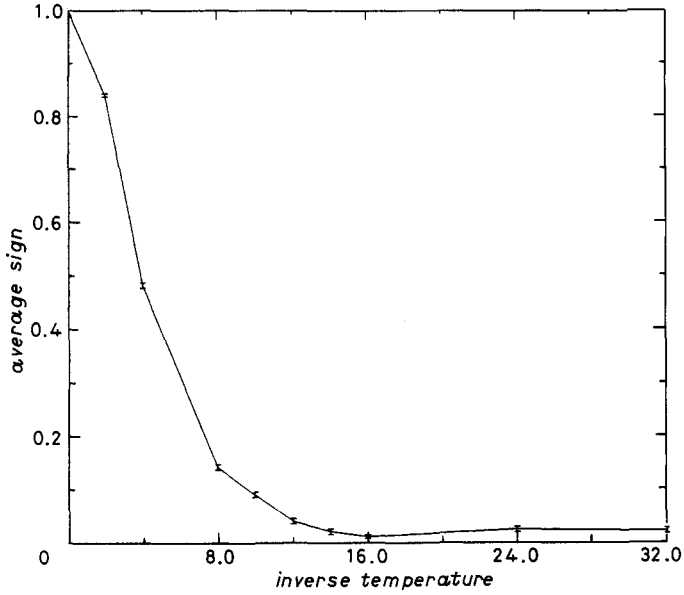

Fig. 2. – Values of $\langle s \rangle_M$ as a function of the inverse temperature β.

larger than previously thought possible [15]. A detailed study of the properties of 1D or 2D Hubbard model will be presented elsewhere.

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REFERENCES

[1] KALOS M. H., in *Monte Carlo Method in Quantum Physics*, edited by M. H. KALOS, NATO ASI Series (D. Riedel Publ. Co., Dordrecht) 1984, p. 19.
[2] CEPERLEY D. M., in *Recent Progress in Many-Body Theories*, edited by J. G. ZABOLITZKY, M. DE LIANO, M. FORTES and J. M. CLARK (Springer Verlag, Berlin) 1981, p. 262.
[3] BLANKENBECKER R., SCALAPINO D. J. and SUGAR R. L., *Phys. Rev. D*, 24 (1981) 2278.
[4] HIRSCH J. E., *Phys. Rev. B*, 31 (1985) 4403.
[5] MORGENSTERN I. and WORTZ D., *Z. Phys. B*, 61 (1985) 219.
[6] KOONIN S. E., SUGIYAMA G. and FRIEDRIECH H., *Proceedings of the International Symposium Bad Honnef*, edited by K. GOEKE and P. G. GREINHARD (Springer Verlag, Berlin) 1982, p. 214.
[7] ANDERSON P. W., *Science*, 235 (1987) 1196.
[8] FEST M. D., FLECK J. A. and STEIGER A., *J. Comp. Phys.*, 47 (1982) 412.
[9] DE RAEDT H., *Comp. Phys. Rep.*, 7 (1987) 1.
[10] PARISI G. and YOUGSHI W., *Scientia Sinica*, 24 (1981) 483.
[11] GUNSTEREN W. F. and BERENDSEN H. J., *Mol. Phys.*, 45 (1982) 637.
[12] SORELLA S., to be published.
[13] LIEB E. H. and WU F. Y., *Phys. Rev. Lett.*, 20 (1968) 1445.
[14] PAROLA A., private communication.
[15] SORELLA S., TOSATTI E., BARONI S., CAR R. and PARRINELLO M., *Int. J. Mod. Phys. B*, 1 (1988) 993.