Since

$$(\Delta p)^2-(\Delta mu)^2=E\left(\left(\frac{p_+(t)+p_-(t)}{2}\right)^2\right)-E(p_+(t))E(p_-(t))$$
$$=\int dx\,\rho(x,t)\left(\frac{\partial S(x,t)}{\partial x}\right)^2-\left(\int dx\,\rho(x,t)\frac{\partial S(x,t)}{\partial x}\right)^2, \tag{23}$$

we can conclude that

$$(\Delta p)^2=(\Delta mv)^2+(\Delta mu)^2. \tag{24}$$

In particular,

$$\Delta p\geq\Delta mu. \tag{25}$$

Namely, the Heisenberg position-momentum uncertainty relations

$$[\langle\psi(t),x^2\psi(t)\rangle-\langle\psi(t),x\psi(t)\rangle^2]^{1/2}\times[\langle\psi(t),p^2\psi(t)\rangle-\langle\psi(t),p\psi(t)\rangle^2]^{1/2}\geq\hbar/2 \tag{26}$$

can be traced back to the position–osmotic velocity uncertainty relation

$$\{E(q^2(t))-[E(q(t))]^2\}^{1/2}\left[E\left(\left(\frac{p_+(t)-p_-(t)}{2}\right)^2\right)\right]^{1/2}\geq\frac{\hbar}{2} \tag{27}$$

for the stochastic process $q(t)$ associated with the wave function $\psi(x,t)$ in the sense of Nelson.

As a final physical remark, we wish to observe that out of the two terms of the decomposition (24) of the root mean square deviation of the quantum-mechanical momentum there is a part due to the current velocity and a part due to the osmotic velocity; it is just the osmotic term that forces the position-momentum uncertainty.

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Stochastic Method for the Numerical Study of Lattice Fermions

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A new stochastic method for the numerical study of lattice fermions is presented. Its efficiency is demonstrated on a field-theoretic model in four dimensions with coupled boson and fermion degrees of freedom. The exact fermion propagator is calculated and agrees very accurately with the numerical results of the stochastic procedure on finite lattices of 10^4 and $8^3\times 16$ sites, respectively. The contribution of fermionic vacuum polarization to mass renormalization is evaluated with precision. The method is directly applicable to quantum chromodynamics.

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During the last twelve months we have witnessed considerable effort to develop Monte Carlo methods for the numerical study of quantum systems with fermionic degrees of freedom. This outstanding problem is of great importance for applications in quantum field theories, condensed matter physics, and nuclear physics.

Previous techniques[1-9] were slow when a very large number of fermionic degrees of freedom were involved, since the computational time re-

quired for a Monte Carlo sweep through the lattice was always proportional to the square of the crystal volume,[10] or even worse.

Recently, this problem was solved by Hirsch *et al.* in one space and one time dimension.[11] They follow the evolution of fermion world lines along the Euclidean time direction with an update time independent of the lattice volume. The method is fast and efficient in applications. The generalization of this ingenious idea to higher dimensions is desirable.

I will follow here the more standard strategy and work directly with a new effective action of the boson fields when the fermionic degrees of freedom are integrated out. Though the effective action becomes nonlocal in the presence of the fermion determinant, the new procedure maintains the efficiency of the standard Monte Carlo technique where the update time on a site is independent of the lattice volume. The method is applicable in any number of dimensions.

For a general presentation, I will consider now the Euclidean action

$$S = S_0(U) + \sum_{ij} \bar{\psi}_i M_{ij}(U) \psi_j \qquad (1)$$

in four dimensions. It describes the interaction of a boson field U_i with a fermion field ψ_i, and the subscripts on the fields refer to the lattice points. Spin and internal symmetry indices are suppressed, for simplicity. The matrix $M_{ij}(U)$ designates both kinetic and mass terms for the fermion field, and couplings to the boson field. $S_0(U)$ describes the pure bosonic part of the Euclidean action. It is important to note that most of the interesting models in quantum field theory, condensed matter physics, and nuclear physics can be brought to a bilinear form in the fermion fields.

The fermion Green's functions can be calculated by inserting sources into the path integral

$$Z(\bar{\eta},\eta) = \int \mathfrak{D}\bar{\psi}\, \mathfrak{D}\psi\, \mathfrak{D}U \exp[-S + \textstyle\sum_i (\bar{\eta}_i \psi_i + \bar{\psi}_i \eta_i)]. \qquad (2)$$

By taking the functional derivatives and integrating out the Grassman variables, the fermion correlation function can be written as

$$\langle \bar{\psi}_i \psi_j \rangle = \frac{\delta^2}{\delta\eta_i\, \delta\bar{\eta}_j} \ln Z(\bar{\eta},\eta)\Big|_{\bar{\eta}=\eta=0} = Z^{-1} \int \mathfrak{D}U\, M_{ij}^{-1}(U) \exp[-S_{\mathrm{eff}}(U)], \qquad (3)$$

where Z is the partition function (normalization integral) of the boson-fermion system. The effective action is given by

$$\exp[-S_{\mathrm{eff}}(U)] = \det[M(U)] \exp[-S_0(U)], \qquad (4)$$

and I assume, for simplicity only, that the fermion determinant has positive sign.

I apply now the Metropolis Monte Carlo method to the evaluation of the functional integral in Eq. (3). Other Euclidean Green's functions can be treated similarly.

It was shown by Scalapino and Sugar,[2] and by Fucito *et al.*,[1] that a local change $U \to U + \delta U$ implies

$$\frac{\exp[-S_{\mathrm{eff}}(U+\delta U)]}{\exp[-S_{\mathrm{eff}}(U)]} = \det[1 + M^{-1}(U)\delta M(U)] \times \frac{\exp[-S_0(U+\delta U)]}{\exp[-S_0(U)]}. \qquad (5)$$

With local boson-fermion coupling the nontrivial change δM in the fermion matrix is restricted to the neighborhood of the updated lattice site. Consequently, we need only a few inverse elements of the large matrix M in each Metropolis step.

At that point I depart from standard procedures. Since the results of a Monte Carlo calculation are always subject to some statistical inaccuracy, it is reasonable to evaluate the decision-making step stochastically. The error analysis becomes subtle,[12] but I am not concerned with it here. I will calculate the inverse matrix elements of M by some modification of a stochastic method which was first suggested by J. von Neumann and S. M. Ulam, but never published by them.[13] It is a very efficient method for the approximate summation of the von Neumann series defined by the inverse of the operator M.

Assume that the inverse of a matrix M of order m is desired and let $H = I - M$, where I is the unit matrix. For the method to be applicable, it is necessary and sufficient that the eigenvalues of the matrix $\tilde{H}_{ij} = |H_{ij}|$ are less than 1 in absolute value. Note that the above condition can always be arranged by proper normalization. The matrix elements $(M^{-1})_{ij}$ are given by the solutions of the linear system of equations $Mx = b$, with unit driving vectors on the right-hand side. This equation is equivalent to $(2/\mu)M^{\dagger}Mx = (2/\mu)M^{\dagger}b$, where μ is the first norm of the matrix $M^{\dagger}M$. The driving vector $(2/\mu)M^{\dagger}b$ may be decomposed into a linear combination of unit vectors and, with the replacement $M \to (2/\mu)M^{\dagger}M$, the method applies even in the worst case.

I decompose the matrix element H_{ik} into $H_{ik} = P_{ik}R_{ik}$ with the restriction that $P_{ik} > 0$ and

$\sum_{r=1}^{m} P_{ir} < 1$ for all values of i. Consider a random walk on the domain of integers $1,2,\ldots,m$. The walk begins at some selected point i and proceeds from point to point with the transition probabilities P_{ik}. The walk stops after k steps at some point s_k with the stop probability $P_{s_k} = 1 - \sum_{r=1}^{m} P_{s_k r}$. When the walk stops, a score S_{ij} is registered for the elements in the ith row of the inverse matrix. It is defined by the product of the residues $R_{s_r s_{r+1}}$ along the trajectory $i \to s_1 \to s_2 \to \ldots \to s_k = j$ divided by the stop probability P_j:

$$S_{ij} = \begin{cases} 0 & \text{if } s_k \neq j \\ R_{is_1} R_{s_1 s_2} \cdots R_{s_{k-1} j} P_j^{-1} & \text{if } s_k = j . \end{cases} \quad (6)$$

I will prove that the expectation value of the random variable S_{ij} is $(M^{-1})_{ij}$. Indeed, the probability of a walk to follow some trajectory $i \to j$ and to stop at j is $P(i \to j)P_j = P_{is_1} P_{s_1 s_2} \cdots P_{s_{k-1} j} \times P_j$. The expected score is given by the sum over all trajectories from i to j:

$$\langle S_{ij} \rangle = \sum_{i \to j} P(i \to j) P_j S_{ij} = \sum_{i \to j} P(i \to j) R(i \to j), \quad (7)$$

where $R(i \to j)$ is the product of the residues along the trajectory. Since $P_{ij} R_{ij} = H_{ij}$, Eq. (7) is recognized as the von Neumann series expansion for $M^{-1} = (I - H)^{-1}$. The term δ_{ij} in the von Neumann series is generated by walks which stop immediately.

It is easy to prove that the variance σ_{ij}^2 of the random variable S_{ij} is given by

$$\sigma_{ij}^2 = (Q^{-1})_{ij} P_j^{-1} - (M^{-1})_{ij}^2 ,$$

where $Q = (I - K)^{-1}$ with $K_{ij} = H_{ij} R_{ij}$. The variance of S_{ij} is finite, provided the von Neumann series for $Q = (I - K)^{-1}$ exists.

The statistical error on $(M^{-1})_{ij}$ is given by $\sigma_{ij}/\sqrt{N}$ for N walks which all begin at point i. For a given statistical accuracy in the decision-making step of the Metropolis procedure, the required number of walks does not depend on the size of the matrix. Therefore, the update time in this stochastic procedure is independent of the lattice volume. My tests involved matrices of the order of 10^4, or larger.

I will now modify the von Neumann–Ulam algorithm for better efficiency in fermionic Monte Carlo procedures. It is easy to realize that during a walk which started at point i, one can register the product of residues at each pass through the point j. I define a new random variable $\tilde{S}_{ij}$ as the sum of the products of residues, adding a new term to the score at each pass through the point j. The stop probabilities are eliminated from the random variable $\tilde{S}_{ij}$, but they still govern the average length of a walk.

It is straightforward to show that $\langle S_{ij} \rangle = \langle \tilde{S}_{ij} \rangle$ when the stop probability P_j is positive. I have also proved[12] that the expectation value $\langle \tilde{S}_{ij} \rangle$ is equal to $(M^{-1})_{ij}$ when the stop probability P_j vanishes. The original method does not apply in this case.

In order to compare efficiencies, I choose a simple case when all $R_{ij} = 1$ and P_j is positive. A necessary and sufficient condition[12] for the variance of the random variable $\tilde{S}_{ij}$ to be smaller than σ_{ij}^2 is $P_j < e_j/(2 - e_j)$, where e_j designates the escape probability from the point j. In practice, this condition is enforced by the nature of the fermion problem, and the modified method is much more efficient.

In the special case when all stop probabilities vanish, one has to stop by fiat. Some bias is introduced then, since the von Neumann series is truncated after a finite number of terms. The modification described above is probably known to some experts on stochastic methods and the special case when the random walk is stopped by fiat appears in the work of Bakhvalov.[14]

I tested my stochastic fermion method on a four-dimensional boson-fermion model which was first suggested by Scalapino and Sugar.[2,7] The fermion matrix M in Eq. (1) is specified now as

$$M_{ij} = -\Delta_{ij} + (m^2 + g U_i^2)\delta_{ij} , \quad (8)$$

where U_i and ψ_i are a scalar boson field and a spinless fermion field, respectively. Δ_{ij} defines the Laplacian operator on the lattice, m is the bare fermion mass in lattice spacing units, and g designates the dimensional boson-fermion coupling constant. The functional integral is calculable analytically in this model,[2] and one finds

$$D(i - j) = \langle \bar{\psi}_i \psi_j \rangle = (-\Delta + m^2 + \tfrac{1}{2} g)_{ij}^{-1} . \quad (9)$$

The fermion-boson interaction generates a mass term dynamically, and the renormalized fermion mass is given by $m_r = (m^2 + \frac{1}{2} g)^{1/2}$.

Some results of my calculations are presented in Fig. 1. The complete fermion mass was generated dynamically with the choice $m = 0$. The agreement of the numerical points with the exact analytic form is very satisfactory (the statistical errors are practically not visible on the logarithmic plot). The quenched approximation,[15-17] where one neglects the fermionic vacuum polarization effects from the fermion determinant in

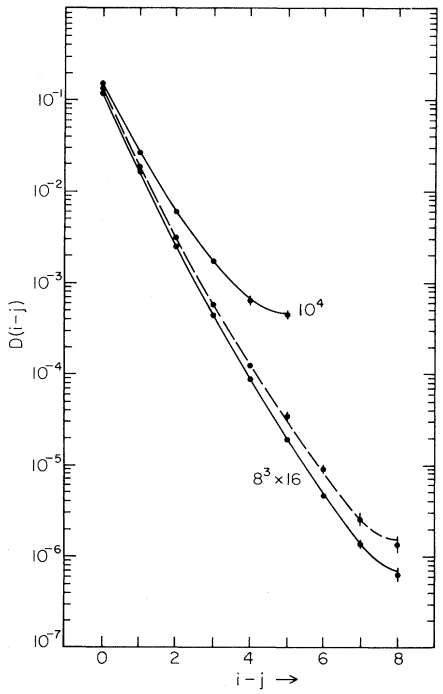

FIG. 1. Some numerical results on the fermion correlation function compared with exact calculations. $D(i-j)$ is depicted for a lattice of $8^3\times 16$ sites with periodic boundary conditions and coupling constant $g = 2.6a^{-2}$ (in the actual calculations the lattice spacing a was set to unity). The free fermion propagator, with renormalized mass $m_r{}^2 = 1.3a^{-2}$ on the same lattice size, is represented by the solid line. Results are also presented for a lattice of 10^4 sites with $m_r{}^2 = 0.25a^{-2}$. The dashed line is the fit of a free fermion propagator of mass $m_q{}^2 = 1.02a^{-2}$ to the results of the quenched approximation on the $8^3\times 16$ periodic lattice with $g = 2.6a^{-2}$ and $m = 0$. The continuous curves for the exact propagators are drawn to guide the eye.

the effective action, is also presented in Fig. 1. The contribution of the fermion loops is clearly seen and accurately calculated: $m_q{}^2/m_r{}^2 = 0.78$.

The speed and efficiency of my stochastic method is very promising. It took only about 3 h on a VAX 11/780 to calculate the complete fermion propagator on the $8^3\times 16$ lattice, with relative errors which are only a few percent even for a separation of eight links along the fourth direction. Details of the numerical results will be published elsewhere.[12]

Some work is in progress now on the numerical solution of quantum chromodynamics,[18] and the Hubbard model in two and three spatial dimensions.[19] I am also working on further theoretical improvements in the stochastic method.

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