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Method for Performing Monte Carlo Calculations for Systems with Fermions

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A method is presented for carrying out Monte Carlo calculations for field theories with fermion degrees of freedom. As an example of this technique, results are given for a simple one-dimensional model.

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Recently Monte Carlo calculations have been used to study a variety of field-theory problems in condensed matter and high-energy physics. To date this technique has been applied only to boson systems. The difficulty with treating fermions is that in the path-integral formulation of field theory, they are represented by anticommuting c-number fields which do not lend themselves to direct numerical calculations. However, Fucito, Marinari, Parisi, and Rebbi have just made a very interesting proposal for performing Monte Carlo calculations of systems with fermions.[1] In this note we present an alternative, but closely related, method for carrying out such calculations. We illustrate our approach by studying a simple one-dimensional field-theory model.

Let us consider the interaction of a boson field A_i with a fermion field ψ_i. We work on a lattice and the subscripts on the fields refer to the lattice points. For simplicity we suppress spin and internal-symmetry labels. We take the Euclidean action to be

$$S = S_0(A) + \sum_{i,j} \bar{\psi}_i O_{ij}(A) \psi_j . \tag{1}$$

The matrix $\underline{O}$ contains the kinetic-energy terms for the fermion field as well as the coupling terms between the boson and fermion fields. It is crucial that the action be bilinear in the fermion field. Most systems of interest are of this form or can be reduced to it by the introduction of auxiliary fields.

In the usual way, we start by integrating out the fermion field. For example, the fermion correlation function can be written as

$$\begin{aligned}\langle \bar{\psi}_i \psi_j \rangle &= z^{-1} \int \delta A \, \delta\bar{\psi} \, \delta\psi \exp(-S) \bar{\psi}_i \psi_j \\ &= z^{-1} \int \delta A \exp[-S_0(A)] [\underline{O}^{-1}(A)]_{ij} \det[\underline{O}(A)],\end{aligned} \tag{2}$$

where z is the normalization integral

$$\begin{aligned} z &= \int \delta A \, \delta\bar{\psi} \, \delta\psi \exp(-S) \\ &= \int \delta A \exp[-S_0(A)] \det[\underline{O}(A)]. \end{aligned} \tag{3}$$

Clearly, all quantities of interest can be obtained from functional integrals with respect to A with an effective action given by

$$\exp[-S_{\text{eff}}(A)] = \exp[-S_0(A)] \det[\underline{O}(A)]. \tag{4}$$

Of course, Eq. (4) makes sense only if $\det[\underline{O}]$ has a definite sign.

Let us now imagine carrying out the functional integral over A with use of the Metropolis Monte Carlo method.[2] We wish to bring the system into equilibrium with the probability of any field configuration A being proportional to $\exp[-S_{\text{eff}}(A)]$. To this end we repeatedly generate random chang-

es in A, $A \to A + \delta A$, which in turn generate changes in the matrix $\underline{O}$, $\underline{O}(A) \to \underline{O}(A + \delta A) \equiv \underline{O}(A) + \delta\underline{O}$. We accept or reject such a change depending on whether the quantity $\exp[-S_{\text{eff}}(A + \delta A) + S_{\text{eff}}(A)]$ is greater or less than a random number between 0 and 1. To make this comparison we must evaluate the ratio of determinants

$$\Delta = \det[\underline{O}(A + \delta A)]/\det[\underline{O}(A)] = \det[1 + \underline{G}(A)\delta\underline{O}], \quad (5)$$

where $\underline{G}(A) = \underline{O}^{-1}(A)$. At first glance, the calculation of Δ appears to be prohibitively lengthy because on a lattice with N sites, $\underline{G}$ and $\delta\underline{O}$ are $N \times N$ matrices.

Fucito *et al.*[1] suggest that we restrict ourselves to small variations in A, so that $\delta\underline{O}$ will be small. Then $\Delta \simeq \mathrm{tr}(\underline{G}\,\delta\underline{O})$. They further suggest that the elements of $\underline{G}$ can be obtained from a Monte Carlo calculation by introducing an auxiliary boson field φ governed by an action

$$S_\varphi = \sum_{i,j} \varphi_i^* O_{ij} \varphi_j. \quad (6)$$

It would appear that the major difficulty with the proposal of Fucito *et al.* is the restriction to small variations in A. One can easily imagine systems with more than one local minimum in $S_{\text{eff}}(A)$ which it would be difficult to leave by making only a succession of small variations in A. However, we can eliminate this restriction. In practical Monte Carlo calculations, one sweeps through the lattice, making a change in A at one lattice site (or on one lattice link) at a time. In a theory with local couplings a change in A at the site l will induce a change in $O_{ij}(A)$ only for values of i and j in the vicinity of l. By writing Δ in the form $\Delta = \exp[\mathrm{tr}\ln(1 + \underline{G}\,\delta\underline{O})]$ and expanding the logarithm as a power series in $\underline{G}\,\delta\underline{O}$, we see that if δO_{ij} is nonzero only for L values of i and of j, then in order to obtain Δ, we need only calculate the determinant of an $L \times L$ matrix. In particular, for nonderivative couplings, a change in A at the site l will induce a change in $\underline{O}$ of the form $\delta O_{ij} = c\delta_{il}\delta_{jl}$, so that

$$\Delta = 1 + cG_{ll}(A). \quad (7)$$

Thus, the restriction to small changes in A is eliminated.

At this point one could simply adopt the proposal of Fucito *et al.* and obtain the needed elements of $G_{ij}(A)$ by a Monte Carlo calculation. However, it may be useful to take further advantage of the locality of $\delta\underline{O}$. Suppose one knows $\underline{G}$ at some particular field configuration A. Then

$$\underline{G}(A + \delta A) = \underline{G}(A) - \underline{G}(A)(\delta\underline{O})\underline{G}(A + \delta A). \quad (8)$$

If $\delta\underline{O}$ has only L^2 nonzero matrix elements, then Eq. (8) can be solved for $\underline{G}(A + \delta A)$ simply by inverting an $L \times L$ matrix. For our special case of nonderivative coupling,

$$G_{ij}(A + \delta A) = G_{ij}(A) - G_{il}(A)G_{lj}(A)c[1 + cG_{ll}(A)]^{-1}. \quad (9)$$

An extreme procedure would be to start the calculation with a trivial field configuration, such as a constant A field, so that $\underline{G}(A)$ could be obtained analytically. Then update G_{ij} each time A is changed with use of the exact formula of Eq. (8) or Eq. (9). We have applied this procedure to the simple one-dimensional model defined by

$$S_0 = \sum_{i=1}^{N} A_i^2, \quad O_{ij}(A) = D_{ij} + (m + gA_i^2)\delta_{ij}, \quad (10)$$

where the derivative matrix, D_{ij}, has $D_{ii} = 2$, $D_{i,i+1} = D_{i+1,i} = D_{1,N} = D_{N,1} = -1$, and all other elements zero. In Table I, we compare typical results of our Monte Carlo calculation of the fermion correlation function with the exact answer, which is easily seen to be

$$c(i - j) = \bar{\psi}_i \psi_j = [\underline{D} + (m + \tfrac{1}{2}g)\underline{I}]_{ij}^{-1}. \quad (11)$$

The results shown in Table I are for $m = g = 1$, with $N = 10$. They were obtained by making 1100 passes through the lattice. The first 100 were to allow the system to reach equilibrium; thereafter, data were collected every tenth pass.

Although the above procedure worked extremely well for our one-dimensional model, we do not expect it to be directly applicable to multidimensional systems. It simply takes too long to update the $N \times N$ matrix $G_{ij}(A)$, even by so simple

TABLE I. The fermion correlation function defined in Eq. (11) for $g = m = 1$. In column 1 we give results of the Monte Carlo calculation described in the text; and in column 2, the exact result.

	Monte Carlo	Exact
$c(0)$	0.3492	0.3482
$c(1)$	0.1099	0.1093
$c(2)$	0.0346	0.0343
$c(3)$	0.0110	0.0109
$c(4)$	0.003 75	0.003 71
$c(5)$	0.002 15	0.002 12

a formula as Eq. (9). We can, however, imagine dividing the lattice into p blocks with N/p sites per block. As we sweep through the lattice, updating A at each site, we can calculate G_{ij} within a block by a Monte Carlo calculation as suggested by Fucito *et al.*, but at each step within the block we can update G_{ij} by Eq. (8) or Eq. (9). We will thus have to make p, rather than N, Monte Carlo calculations during each sweep through the lattice, and in our recent updating of G_{ij} we will only have to work with an $(N/p)\times(N/p)$ matrix. The optimum choice for p will, of course, depend on the system being studied.

Finally, we remark that it may be possible to find alternative methods for calculating the matrix elements of $\underline{G}$. For example, consider the equation

$$\underline{O}\,\underline{g}=\underline{h}, \tag{12}$$

where $\underline{g}$ and $\underline{h}$ are N-component column vectors. If we choose the elements of h to be $h_i=\delta_{ij}$, then $g_i=G_{ij}$. Since $\underline{O}$ will generally be a very sparse matrix, it may be possible to solve for the g_i rapidly. For example, in the model which we have discussed, the elements of $\underline{g}$ satisfy a three-term recursion relation which can be solved in $2N$ steps, a considerable saving over the N^2 steps necessary to update the matrix $\underline{G}$ by Eq. (9). Alternatively, one may be able to solve Eq. (12) rapidly by relaxation methods.

Although it is far from clear that we have arrived at the optimal procedure, it does seem certain that these techniques can be applied to a number of interesting systems, particularly lower-dimensional ones in condensed-matter physics.

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[1]F. Fucito, E. Marinari, G. Parisi, and C. Rebbi, CERN Report No. CERN-TH-2960 (to be published).

[2]N. Metropolis, A. W. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. 21, 1087 (1953).