

A PROPOSAL FOR MONTE CARLO SIMULATIONS OF FERMIONIC SYSTEMS

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We suggest a possible extension of the Monte Carlo technique to systems with fermionic degrees of freedom. We study in detail the application to an elementary example.

1. Introduction

Monte Carlo simulations have recently emerged as one of the most powerful methods for obtaining information on pure gauge theories [1]. If this technique is to be used for a direct computation of properties of known particles, however, the effect of fermions must be properly included.

In the Feynman path integral formulation, fermions are described by anticommuting variables. N anticommuting variables span an algebra with 2^N generators: even for fairly small values of N , the amount of space needed to store a single element of this algebra exceeds by far the memory capacity of any possible computer.

Anticommuting variables must be avoided in computer simulations. In many physically interesting cases, this can be accomplished by using the Matthews-Salam

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formula. Let the euclidean action be given by

$$S[\bar{\psi}, \psi, A] = \sum_{i,j} \bar{\psi}_i \Delta_{ij}[A] \psi_j + S_0[A], \quad (1.1)$$

where $\bar{\psi}_i$ and ψ_i ($i = 1, N$) are the fermionic fields and A stands for the bosonic fields. It is crucial that the action be bilinear in the fermionic variables (quite often the action is of this form or may be reduced to it by introducing auxiliary fields). Then the integration over the fermionic degrees of freedom can be done analytically:

$$\int d[\bar{\psi}] d[\psi] \exp\{-S[\bar{\psi}, \psi, A]\} = \det\{\Delta[A]\} \exp\{-S_0[A]\},$$

$$\int d[\bar{\psi}] d[\psi] \bar{\psi}_i \psi_j \exp\{-S[\bar{\psi}, \psi, A]\} = \{\Delta[A]\}^{-1}_{ji} \det\{\Delta[A]\} \exp\{-S_0[A]\}. \quad (1.2)$$

Similar results can be obtained for higher-order Green functions.

If $\det\{\Delta[A]\}$ does not change sign as a function of A (e.g., $\Delta[A]$ is a positive definite operator or its eigenvalues always have even multiplicity), it can be absorbed into the action, producing an effective action for the bosonic field A :

$$S_{\text{eff}}[A] = S_0[A] - \text{Tr} \ln \Delta[A]. \quad (1.3)$$

All of this is well known. In principle, one could do Monte Carlo simulations for $S_{\text{eff}}[A]$: however, the exact computation of the determinant is too slow (it requires N^3 steps). In this paper we propose a simple technique to evaluate approximately the determinant (more precisely the ratio of two determinants), which requires an acceptable amount of computer time. In sect. 2, we describe the method; in sect. 3, we apply it to a simple system, and in sect. 4 we present a few short remarks on the connection of this procedure with equations of the Langevin type.

2. The introduction of pseudofermions

For the reader's convenience, we recall the principles of Monte Carlo simulations [1, 2]. The aim is to compute

$$\langle f[A] \rangle \equiv \frac{\int d[A] f[A] \exp\{-S[A]\}}{\int d[A] \exp\{-S[A]\}}. \quad (2.1)$$

As a starting point one constructs an algorithm which, given the configuration A , generates a new, trial configuration \tilde{A} , according to a definite probability distribution $P(A \rightarrow \tilde{A})$. P must satisfy $P(A \rightarrow \tilde{A}) = P(\tilde{A} \rightarrow A)$. If A is an unconstrained real variable, the simplest algorithm consists in adding to A a random variable with symmetric distribution.

A sequence of configurations $A^{(i)}$ is then generated in the following way. Starting from $A = A^{(i)}$, the new, trial configuration \tilde{A} is determined and a random number x is extracted with uniform probability distribution over the unit interval. If

$$\exp\{- (S[\tilde{A}] - S[A])\} > x, \tag{2.2}$$

$A^{(i+1)}$ is set equal to \tilde{A} ; otherwise, $A^{(i+1)}$ is set equal to the old configuration A . (In other words, if the new configuration leads to lower action, the change $A \rightarrow \tilde{A}$ is always accepted; if not, it is accepted with the conditional probability $\exp\{-(S[\tilde{A}] - S[A])\}$.) This guarantees that the sequence eventually reaches a regime of statistical equilibrium, where the probability of encountering any definite configuration A is proportional to $\exp\{-S[A]\}$. It follows

$$\langle f[A] \rangle = \lim_{k \rightarrow \infty} \left(\frac{1}{k} \sum_{i=1}^k f[A^{(i)}] \right). \tag{2.3}$$

Eq. (2.3) holds independently of the choice of probability distribution $P(A \rightarrow \tilde{A})$; however, if this choice is not “appropriate”, the convergence of the right-hand side of eq. (2.3) may be very slow.

To apply this algorithm to

$$S_{\text{eff}}[A] = S_0[A] - \text{Tr} \ln \{ \Delta[A] \},$$

we must compute the ratio of two determinants. A substantial simplification occurs if we choose $P(A \rightarrow \tilde{A})$ so that \tilde{A} is close to A . Neglecting terms corresponding to higher powers of $(\tilde{A} - A)$, we obtain

$$S_{\text{eff}}[\tilde{A}] - S_{\text{eff}}[A] = S_0[\tilde{A}] - S_0[A] - \sum_{i,j} (\Delta^{-1})_{ji} \Delta'_{ij} (\tilde{A} - A), \tag{2.4}$$

where $\Delta'_{ij} = \delta \Delta_{ij} / \delta A$.

Unfortunately, the computation of $(\Delta^{-1})_{ji}$ is also impractical: our suggestion is to compute $(\Delta^{-1})_{ji}$ approximately using a Monte Carlo technique. Indeed, if Δ is a

positive operator, we can write

$$\begin{aligned}
 (\Delta^{-1})_{ji} &= \langle \bar{\phi}_i \phi_j \rangle \\
 &= \frac{\int d[\bar{\phi}] d[\phi] \bar{\phi}_i \phi_j \exp\{-\sum_{i,j} \bar{\phi}_i \Delta_{ij} \phi_j\}}{\int d[\bar{\phi}] d[\phi] \exp\{-\sum_{i,j} \bar{\phi}_i \Delta_{ij} \phi_j\}}, \tag{2.5}
 \end{aligned}$$

where $\bar{\phi}_i, \phi_i$ are complex bosonic fields which will be called pseudofermions. $\bar{\phi}_i$ and ϕ_i interact like the fermions but are ordinary numbers.

[If Δ is real symmetric, real bosonic fields ϕ_i are sufficient. Eq. (2.5) is replaced by

$$\begin{aligned}
 (\Delta^{-1})_{ji} &= \langle \phi_i \phi_j \rangle \\
 &= \frac{\int d[\phi] \phi_i \phi_j \exp\{-\frac{1}{2} \sum_{i,j} \phi_i \Delta_{ij} \phi_j\}}{\int d[\phi] \exp\{-\frac{1}{2} \sum_{i,j} \phi_i \Delta_{ij} \phi_j\}} \tag{2.6}
 \end{aligned}$$

and all subsequent formulae are changed accordingly.]

The final prescription is the following. We construct Monte Carlo simulations for the coupled system of $A, \bar{\phi}$ and ϕ very much as in the standard application of the method, but with two major differences: for each upgrading of the bosonic field A , the pseudofermionic variables $\bar{\phi}$ and ϕ are upgraded n times. When we upgrade the fields, different actions are used: these are, respectively,

$$S_{\bar{\phi}, \phi} = \sum_{i,j} \bar{\phi}_i \Delta_{ij} [A] \phi_j, \tag{2.7}$$

$$S_A = S_0[A] - \overline{\sum_{i,j} \bar{\phi}_i \phi_j \Delta_{ij} [A]}, \tag{2.8}$$

where the long bar denotes the average over the last n upgradings of the pseudofermionic fields.

For large n , the pseudofermionic dynamics is much faster than the bosonic one, which is relatively slow: $\langle \bar{\phi}_i \phi_j \rangle$ is very near to $\overline{\bar{\phi}_i \phi_j}$. Neglecting errors proportional to $(\tilde{A} - A)^2$, the correct results are obtained for n going to infinity.

This method reproduces the functional averages of a system with fermions as a limit of Monte Carlo-like simulations; in practice it can work only if not too high values of n are needed to extrapolate to $n \rightarrow \infty$ (the computer time is linear in n). It is hard to estimate theoretically how large n must be; in sect. 3 we show with an explicit example that good results are also obtained for low n . We notice *en passant*

that eqs. (2.7) and (2.8) are easily generalized to the case where N_f fermionic species (flavours) are present, interacting with the A field in an $SU(N_f)$ invariant way. The action for the pseudofermions is not modified; the new bosonic action is

$$S_A = S_0[A] - N_f \sum_{i,j} \overline{\phi}_i \phi_j \Delta_{ij}[A]. \tag{2.9}$$

As expected, for $N_f = 0$ we have no feedback from the pseudofermions on the bosons. With $N_f = -1$ we recover the bosonic theory (-2 charge conjugate bosons are a fermion) and the correct results are obtained also for $n = 1$.

3. A simple example

The ultimate goal would be to apply the method to gauge theories. In this case, A stands for the gauge fields and the fermionic term in the action is $\bar{\psi}(\not{D} + m)\psi$, D being the covariant derivative. The operator $\not{D} + m$ is not positive definite, but we can use the following chain of identities [3]:

$$\begin{aligned} \det[\not{D} + m] &= \left[\det\{(\not{D} + m)^2\} \right]^{1/2} \\ &= \left[\det\{-\not{D} + m\} \det\{\not{D} + m\} \right]^{1/2} = \left[\det\{-\not{D}^2 + m^2\} \right]^{1/2}. \end{aligned} \tag{3.1}$$

The operator $-\not{D}^2 + m^2$ is now positive definite and can be used for the pseudofermionic action. Neglecting colour indices, one would find

$$S_A = \frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \frac{1}{2} N_f \bar{\phi}(m^2 - \not{D}^2)\phi, \tag{3.2}$$

$$S_{\bar{\phi},\phi} = \bar{\phi}(m^2 - \not{D}^2)\phi. \tag{3.3}$$

Having in mind this future application, we have investigated a model with action

$$S = A^2 + \bar{\psi}\psi(1 + gA^2). \tag{3.4}$$

The integrations over bosonic and fermionic degrees of freedom are trivial. One finds

$$\begin{aligned} \langle A^2 \rangle &= \frac{2 + 3g}{4 + 2g}, \\ \langle A^4 \rangle &= \frac{6 + 15g}{8 + 4g}, \\ \langle \bar{\psi}\psi \rangle &= \frac{2}{2 + g}, \\ \langle \delta(A - x) \rangle &\equiv \rho(x) = \frac{2(1 + gx^2)}{\sqrt{\pi}(2 + g)} \exp\{-x^2\}. \end{aligned} \tag{3.5}$$

We have tried to reproduce these results with our modified Monte Carlo simulation. The effective actions for the A and (real) ϕ evolutions are

$$\begin{aligned}
 S_A &= A^2 - 2g\phi^2 A^2, \\
 S_\phi &= \phi^2(1 + gA^2).
 \end{aligned}
 \tag{3.6}$$

n upgradings of the pseudofermion (ϕ) are done for each upgrading of the bosonic field A . The expectation value $\langle \bar{\psi}\psi \rangle$ is given by twice the mean value of ϕ^2 . Using complex ϕ we would have

$$\begin{aligned}
 S_A &= A^2 - g\bar{\phi}\phi A^2, \\
 S_{\bar{\phi},\phi} &= \bar{\phi}\phi(1 + gA^2), \\
 \langle \bar{\psi}\psi \rangle &= \langle \bar{\phi}\phi \rangle.
 \end{aligned}
 \tag{3.7}$$

In the simulation we have set $\tilde{A} = A + \eta$, $\tilde{\phi} = \phi + \eta'$, where η, η' are random variables uniformly distributed over the interval $[-\frac{1}{4}, \frac{1}{4}]$. $\langle \eta^2 \rangle = \frac{1}{48} \ll 1$. With such a small value of $\langle \eta^2 \rangle$ the bulk of the error should come only from the finite value of n . In order to see the n dependence, we have done long runs (250 000 steps for A , 250 000 $\times n$ steps for ϕ) at different values of g and n . In figs. 1 and 2, we show

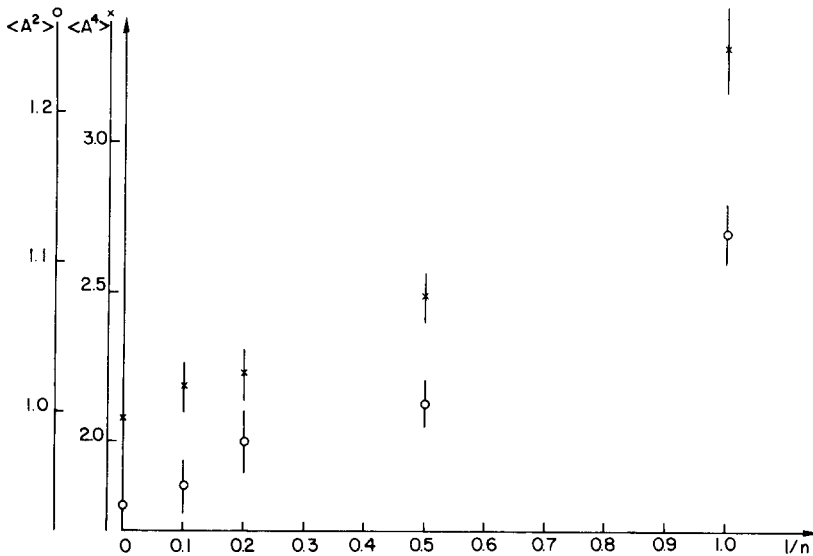


Fig. 1. Values of $\langle A^2 \rangle$ (O) and $\langle A^4 \rangle$ (X) obtained with different numbers n of fermionic steps per bosonic upgrade and $g = 1.6$. Marks at $1/n = 0$ represent the expected exact values.

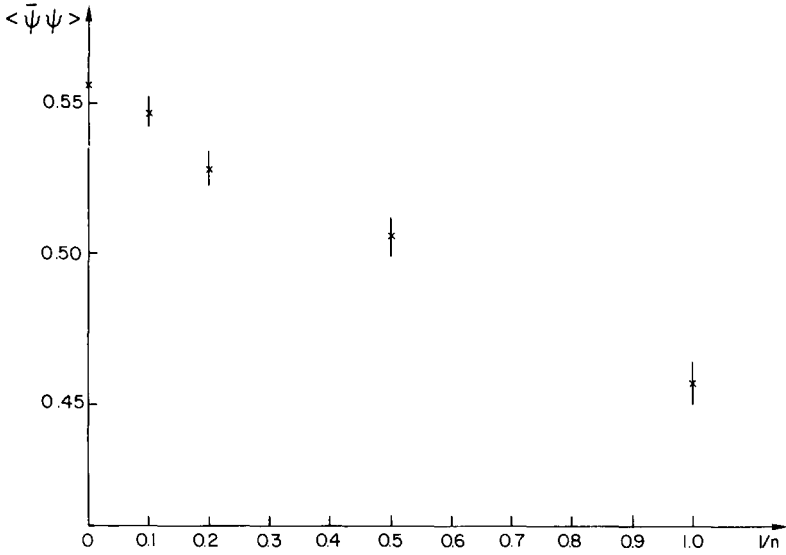


Fig. 2. The same as fig. 1, but values of $\langle \bar{\psi} \psi \rangle$ are reported.

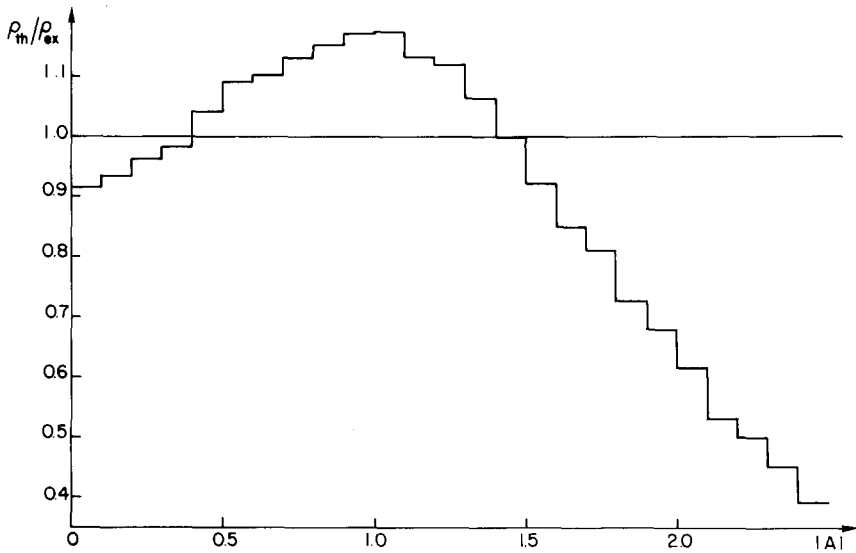


Fig. 3. Ratios of integrated densities $\int_x^{x+\Delta x} \rho_{theor}(x) dx / \int_x^{x+\Delta x} \rho_{exp}(x) dx$ with $n = 1, g = 1.6$.

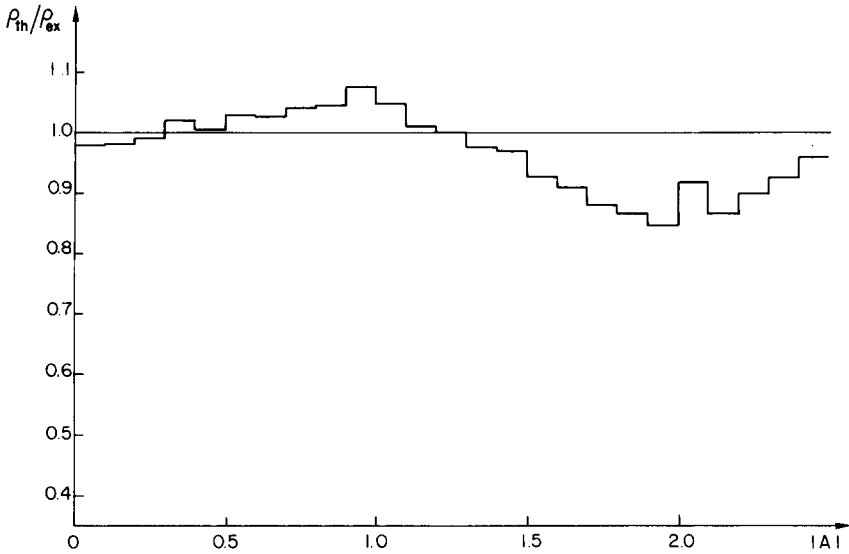


Fig. 4. The same as in fig. 3, but with $n = 5$.

typical results for the moments of A and $\langle \bar{\psi}\psi \rangle$ as functions of n , with $g = 1.6$. In figs. 3 and 4, we display the ratios of the experimental versus theoretical values of the density distributions, integrated over intervals of width 0.1. For large values of $|A|$ (> 2.5), the expected number of events is so small that statistical errors become dominant. In the last interval we reproduce (2.4 – 2.5) only ~ 400 events are expected, so that even for totally uncorrelated events the above statistical error would be $\sim 5\%$.

The results are quite satisfactory. Even for $n = 1$ they appear qualitatively correct and the numbers become rather accurate for $n = 2$. We hope that this gratifying feature will survive more interesting applications.

4. The modified Langevin equation

The disadvantage of the Monte Carlo method is that analytic estimates of the rates of convergence and therefore of the errors are difficult, although one can always use the associated master equation. The Langevin equation is not so efficient for numerical simulations (although its use simplifies the computation of correlation functions), but the analytic study of the solution is easy to do.

For conventional systems the Langevin equation is

$$\dot{A} = -\frac{1}{2} \frac{\partial S}{\partial A} + \eta,$$

$$\langle \eta(t)\eta(t') \rangle = \delta(t - t'), \quad (4.1)$$

η being a random gaussian variable [4]. As in Monte Carlo simulations we have

$$\langle f[A] \rangle = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T f[A(t)] dt. \quad (4.2)$$

If we discretize the time, the Langevin equation becomes very similar to the Monte Carlo procedure. Vice versa, in the limit of very small Monte Carlo steps we obtain the Langevin equation. In this framework, instead of eqs. (3.6), we could write the following stochastic evolution equations:

$$\begin{aligned} \dot{A} &= -A(1 - 2g\phi^2) + \eta_A, \\ \tau \dot{\phi} &= -\phi(1 + gA^2) + \tau^{1/2} \eta_\phi, \\ \langle \eta_A(t) \eta_A(t') \rangle &= \langle \eta_\phi(t) \eta_\phi(t') \rangle = \delta(t - t'), \\ \langle \eta_A(t) \eta_\phi(t') \rangle &= 0. \end{aligned} \quad (4.3)$$

It will be shown elsewhere that in the limit $\tau \rightarrow 0$, one recovers the results for the fermionic system [5]. Everything in this approach is explicit enough to allow precise estimates of the errors.

It is well known that the correlation functions of a bosonic field theory can be computed using the solution of a stochastic differential equation [6, 7]; it is rather remarkable that the correlation functions of a theory with fermions can also be computed using a stochastic differential equation with commuting variables only.

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