Simulation of bosonized lattice fermion theories

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A method is described for converting a fermionic lattice theory into an equivalent Ising-type system which may conveniently be simulated by standard Monte Carlo heat-bath techniques. Fluctuations in physical quantities such as chiral expectation values are found to be controlled. The method is applied to Dirac theory in two space, one time dimensions and excellent agreement is obtained with analytic lattice results.

I. INTRODUCTION

One of the most difficult problems arising in the approach to lattice gauge theory based on Monte Carlo simulation of the Euclidean path integral is the accurate treatment of dynamical fermions. Several approaches have been proposed to date for handling this problem—the pseudofermion method,[1] exact computation of the fermion determinant by finite-rank update,[2] Langevin techniques,[3] or the microcanonical approach[4]—but all are highly computationally intensive. An approach which treated fermionic and bosonic degrees of freedom more symmetrically (thereby avoiding what is in some sense a problem of nested Monte Carlo simulations), would clearly be attractive.

The interconvertibility of fermionic and bosonic fields is well known in connection with the bosonization of fermionic theories in one space, one time dimensions.[5] These techniques have their roots in the Jordan-Wigner representation[6] of anticommuting variables in terms of spin operators. In fact, this representation can also be applied to fermionic fields in higher than one space dimension.[7] In this case, however, it is usually the case that the resulting bosonic action is nonlocal. Recently, there has been an interesting attempt by Gausterer and Lang[8] to apply Langevin techniques to bosonized $(2+1)$-dimensional Dirac theory. Their formulation of the bosonized Hamiltonian contains large relative factors in the matrix elements, however, and this leads to difficulties with fluctuations and slow equilibration, as well as the necessity for taking a highly asymmetrical spatial lattice.

In this paper an alternative formulation of the bosonized Dirac fermion is given which appears to avoid the above difficulties. In this form, the system can be simulated by a heat-bath algorithm in which only the very small fraction of permissible spin configurations (cf. Sec. III) are generated. The fermionic problem is thereby reduced to a simulation of an Ising-type system. The nonlocal string terms contribute to a sign factor which is included in measurements of physical operators but is irrelevant for the updating procedure. Most importantly, one finds that the fluctuations in the physical quantities such as $\langle \bar{\psi}\psi \rangle$ in this approach are controlled, and one is able to obtain excellent agreement with explicit analytic results over a range of bare masses well into the continuum region.

In Sec. II the Jordan-Wigner transformation of $(2+1)$-dimensional Dirac theory is reviewed. Section III describes the Euclidean path integral (strictly speaking, path sum) appropriate for generating finite- or zero-temperature expectations of physical quantities such as the chiral expectation $\langle \bar{\psi}\psi \rangle$. A heat-bath algorithm is explained which generates all and only those spin configurations with nonzero weight in the path integral. Finally, in Sec. IV the results of the simulation are presented and compared with explicit analytic formulas.

II. BOSONIZING LATTICE FERMIONS

To obtain a bosonic transcription of a lattice fermion theory in terms of Ising-type spin variables one may employ the Jordan-Wigner representation[6] of any set of anticommuting variables in terms of spin variables which *commute* at different sites. Namely, if

$$\{\phi_i^\dagger, \phi_j\} = \delta_{ij} \tag{1}$$

one sets

$$\phi_i = \prod_{j<i} (i\sigma_j^3)\sigma_i^- \tag{2}$$

with $\sigma_j^3, \sigma_j^- = (\sigma_j^1 + i\sigma_j^2)/2$ Pauli algebras commuting on separate sites j. The representation (2) presupposes a linear ordering of the fermion fields on any given time slice of the lattice. We shall henceforth consider theories in two space, one time dimensions and order the fermion fields along the canonical path indicated in Fig. 1. In this case, the transcription of a local fermionic theory into spin variables results in nonlocal terms (strings of σ^3 variables) in those parts of the Hamiltonian arising from y links in the original fermionic kinetic energy.

To be specific, let us take a free, massive Dirac theory in $2+1$ dimensions, more or less the simplest case exhibiting the nonlocality. The lattice will be $L_0 \times L \times L$ with spacings a_0, a in the time and spatial directions, respectively. A site on this lattice will be labeled (j_0, j_1, j_2). In terms of dimensionless staggered[9] fermion fields ϕ_{j_1,j_2} the lattice Hamiltonian is (on a particular time slice, suppressing j_0)

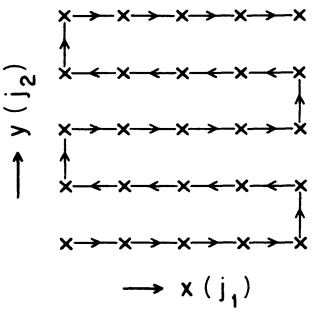

FIG. 1. A canonical ordering of fermions on a two-dimensional lattice.

$$aH=\frac{i}{2}\sum_{j_1,j_2}(-)^{j_1+j_2}\phi^{\dagger}_{j_1j_2}(\phi_{j_1+1,j_2}+\phi_{j_1-1,j_2})$$
$$-\frac{i}{2}\sum_{j_1j_2}\phi^{\dagger}_{j_1j_2}(\phi_{j_1,j_2+1}-\phi_{j_1,j_2-1})$$
$$+\mu_f\sum_{j_1j_2}(-)^{j_1+j_2}\phi^{\dagger}_{j_1j_2}\phi_{j_1j_2}\ . \tag{3}$$

Note that we take free boundary conditions spatially. In (3) $\mu_f=ma$ is the fermion mass in units of the spatial lattice spacing and the $\phi_{j_1j_2}$ are normalized according to

$$\{\phi^{\dagger}_{j_1j_2},\phi_{j_1'j_2'}\}=\delta_{j_1j_1'}\delta_{j_2j_2'}\ . \tag{4}$$

Ordering the $\phi_{j_1j_2}$ along the canonical path indicated in Fig. 1 and performing the replacement (2), the Hamiltonian becomes

$$aH=\tfrac{1}{2}\sum(-)^{j_1}(\sigma^{+}_{j_1j_2}\sigma^{-}_{j_1+1,j_2}+\text{H.c.})$$
$$+\mu_f\sum(-)^{j_1+j_2}\sigma^{+}_{j_1j_2}\sigma^{-}_{j_1j_2}$$
$$+\tfrac{1}{2}\sum(\sigma^{+}_{j_1j_2}\sigma^{-}_{j_1,j_2+1}+\text{H.c.})\Sigma_{j_1j_2}\ . \tag{5}$$

The string variable $\Sigma_{j_1j_2}$ is the uncanceled product of σ^3 operators along the canonical path connecting the sites (j_1,j_2) and (j_1,j_2+1):

$$\Sigma_{j_1j_2}=(-)^{j_1+1}\prod_{j_1j_2<j<j_1,j_2+1}\sigma^3_j \tag{6}$$

for L odd, and

$$\Sigma_{j_1j_2}=(-)^{j_1+j_2}\prod_{j_1j_2<j<j_1,j_2+1}\sigma^3_j \tag{7}$$

for L even. As we shall see below, the evaluation of $\Sigma_{j_1j_2}$ is only relevant to the measurement procedure, not to the updating of the spin variables, and in practice consumes an ignorable fraction (typically 2–3 %) of the computer time in an actual simulation.

A glance at (5) shows that the equivalent spin Hamiltonian has a rather simple structure: in the representation in which $\sigma^3_{j_1j_2}$ are diagonal, with eigenvalues $s_{j_1j_2}$ (referred to in the following as a spin configuration), the only off-diagonal matrix elements arise from flipping opposite spins on adjacent sites. Moreover, the off-diagonal matrix elements of H, and hence of the transfer matrix for this problem, though real, can have either sign, corresponding to a complex Euclidean action, as noted by Gausterer and Lang.[8]

III. SIMULATION PROCEDURE FOR THE BOSONIZED HAMILTONIAN

We would like to be able to compute quantities such as the chiral expectation

$$\langle\bar{\psi}\psi\rangle=\frac{\text{tr}[\exp(-\beta H)\bar{\psi}\psi]}{\text{tr}[\exp(-\beta H)]}\ , \tag{8}$$

where H is the fermionic Hamiltonian (3), by means of a Monte Carlo simulation of the related bosonic representation (5). Attempts based on Langevin techniques[8] appear to lead to severe difficulties with equilibration and large fluctuations. We shall follow here a heat-bath approach that leads to quite stable averages, which moreover agree with explicit analytic results available for the simple fermionic model of the preceding section.

The simulation of (8) can be accomplished by introducing a Euclidean time spacing a_0 and L_0 time slices. Then one computes ($\beta=a_0L_0$)

$$\langle\bar{\psi}\psi\rangle_{\text{latt}}=\frac{\text{tr}(1-a_0H)^{L_0}\bar{\psi}\psi}{\text{tr}(1-a_0H)^{L_0}}$$
$$=\frac{1}{L^2}\frac{\text{tr}(1-a_0H)^{L_0}\sum(-)^{j_1+j_2}\delta_{s_{0j_1j_2},1}}{\text{tr}(1-a_0H)^{L_0}}\ . \tag{9}$$

In the above formula, the chiral expectation is composed as an average over the zeroth time slice ($j_0=0$). As usual, one inserts a complete set of states $|s_{j_0j_1j_2}\rangle$ on each time slice in order to arrive at a path-integral representation for quantities such as (9). As the factor

$$\langle s_{j_0+1,j_1j_2}\,|\,1-a_0H\,|\,s_{j_0j_1j_2}\rangle \tag{10}$$

in this sum is not necessarily positive, we must separate the sign factor

$$S(s_{j_0j_1j_2})=\prod_{j_0}\text{sgn}\langle s_{j_0+1,j_1j_2}\,|\,1-a_0H\,|\,s_{j_0j_1j_2}\rangle \tag{11}$$

from the magnitude portion which will become the (necessarily positive) Monte Carlo measure:

$$P(s_{j_0j_1j_2})=\prod_{j_0}|\langle s_{j_0+1,j_1j_2}\,|\,1-a_0H\,|\,s_{j_0j_1j_2}\rangle|\ . \tag{12}$$

Of course, because of the trace in (9), we have periodicity:

$$s_{J_0+L_0,j_1j_2}=s_{J_0j_1j_2}\ . \tag{13}$$

Evidently

$$\langle \bar{\psi}\psi \rangle_{\text{latt}} = \frac{\left\langle S(s_{j_0 j_1 j_2}) \sum (-)^{j_1+j_2} \delta_{s_0 j_1 j_2, 1} \right\rangle_P}{\langle S(s_{j_0 j_1 j_2}) \rangle_P} , \qquad (14)$$

where the expectation values on the right-hand side in (14) refer to a Monte Carlo average with respect to the positive measure P given in (12). Note that the nonlocal string factors only contribute to S, not to the measure P, and hence are irrelevant in the update procedure.

Contrary to the widely accepted lore on complex actions, we have found that while fluctuations in the sign factor S [and hence in the numerator and denominator factors in (14)] can be sizable, the ratio (14) determining the physical quantity $\langle \bar{\psi}\psi \rangle$ is much more stable (cf. Sec. IV). A successful simulation depends crucially however on an update procedure which avoids the generation of the very large preponderance of configurations carrying zero weight (essentially, as a consequence of the exclusion principle) in the path integral.

From (5) we see that the only configurations appearing in the path integral over the measure (12) are those in which adjacent time slices are either identical or differ by the reversal of a single active link. A link here is a pair of nearest-neighbor sites on a given time slice; an active link is one where the spins on the two sites are opposite. We reverse the link simply by interchanging the spins.

In a Metropolis-type update procedure[10] one might proceed by reversing each available active link on each time slice in turn and then checking the adjacent time slices to see whether the resulting configuration is a permissible one. This scattershot approach leads to an unacceptably small acceptance rate, however, on the order of a few percent at best. Instead, we shall use a heat-bath update in which a new configuration is selected from the range of all permissible configurations for a particular time slice given the fixed configurations on the adjacent ones. The relative probability for the selection is determined by the weight (12). Thus, an update step amounts to examining a time slice and modifying the configuration on the slice in a way compatible with the adjacent slices (i.e., differing at most by the reversal of a single active link).

The heat-bath procedure is implemented by classifying the relation of each time slice to its neighbors into the five possible categories allowed by the Hamiltonian (5). If s represents a configuration of spins on a given time slice, let $s\{l\}$ be the configuration obtained from s by reversing the active link l. The allowed configurations admit the following possibilities for the time slice being considered and its temporal neighbors:

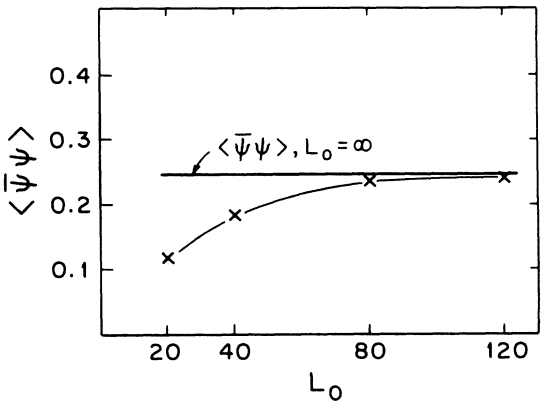

FIG. 2. Large Euclidean time limit of $\langle \bar{\psi}\psi \rangle$.

(1) s,s,s ,

(2) $s,s,s\{l\}$,

(3) $s\{l\},s,s$,

(4) $s\{l\},s,s\{l\}$,

(5) $s\{l\},s,s\{l'\}$.

For example, if the time slice being updated is identical to the preceding and following time slices [situation (1) above], the available new configurations for the central time slice are s and $s\{l\}$ (where l is any active link on s), with relative probabilities $[1-a_0 H_m(s)]^2$ to $(a_0/2)^2$ (for each active link). Here $H_m(s)$ is the mass term part of the Hamiltonian: the coefficient of μ_f in (5). A similar analysis leads to a simple set of rules for each of the situations (2)–(5) in the list above.

IV. RESULTS OF THE MONTE CARLO SIMULATION

The chiral expectation $\langle \bar{\psi}\psi \rangle$ given by (9) has been evaluated using the heat-bath procedure outlined in the preceding section. The Hamiltonian (3) can be solved directly by Fourier and Bogoliubov transformations. For L odd, for example, the result for the ground-state energy is

$$E_0 = -\frac{1}{2} \sum_{p_1,p_2=1}^{L} \left[\cos\left[\frac{\pi p_1}{L+1}\right]^2 + \cos\left[\frac{\pi p_2}{L+1}\right]^2 + \mu_f^2 \right]^{1/2} + \tfrac{1}{2}\mu_f \qquad (15)$$

and the ground-state expectation of $\bar{\psi}\psi$ is

$$-\langle \bar{\psi}\psi \rangle = \frac{1}{2L^2} \sum \frac{\mu_f}{\left[\cos\left[\frac{\pi p_1}{L+1}\right]^2 + \cos\left[\frac{\pi p_2}{L+1}\right]^2 + \mu_f^2 \right]^{1/2}} - \frac{1}{2L^2} . \qquad (16)$$

The spectrum of H is roughly symmetrical, so by taking $a_0 \simeq 1/|E_0|$ we ensure that the limit $L_0 \to \infty$ enhances the ground state over all others via the $(1-a_0 H)^{L_0}$ factor in (9). This is the "low-temperature" limit in which the contribution of excited states is suppressed.

The approach to zero temperature (and hence to pure ground-state expectation values) in the Monte Carlo results is shown in Fig. 2. The system simulated was a 5×5

TABLE I. Estimates of $\langle S \rangle$ and $\langle \bar{\psi}\psi \rangle$ from different runs.

Run	$\langle S \rangle$	$\langle \bar{\psi}\psi \rangle$
1	0.296	0.228
2	0.367	0.244
3	0.212	0.234
4	0.317	0.238
5	0.243	0.233

spatial lattice with dimensionless mass $\mu_f = 0.5$. $\langle \bar{\psi}\psi \rangle$ is shown for the number of time slices $L_0 = 20$, 40, 80, and 120. In the terminology used here, a sweep consists of a single update on each time slice. In other words, the computational requirements for a sweep grow as $O(L_0)$, not $O(L^2 L_0)$. The results presented throughout correspond to averages obtained from five runs of 50 000 sweeps each (about 100 sec on the Cray-XMP for $L_0 = 80$), with 5000 sweeps allowed at the start for thermalization. The initial configuration is one in which $s_{j_0 j_1 j_2} = +1$ for $j_1 + j_2$ odd. The conserved fermion number in this theory corresponds in the spin formulation to the number of up spins, and it is easy to see that all states of nonzero overlap with the exact ground state are generated eventually by action of the Hamiltonian on this starting configuration. The statistical errors in the plotted values of $\langle \bar{\psi}\psi \rangle$ are at most 2–3 % and would hardly be visible on the graph. The systematic (finite-size) discrepancy between the measured $\langle \bar{\psi}\psi \rangle$ and the true ground-state value (16) decreases to about 4% for $L_0 = 80$.

There are strong fluctuations in the sign factor $\langle S \rangle$ defined in (11), and hence in both numerator and denominator of (14). The ratio, however, which is of physical interest, is much more stable. This is clearly seen in Table I, where results for $\langle S \rangle$ and $\langle \bar{\psi}\psi \rangle$ are presented for $\mu_f = 0.5$ and $L_0 = 80$. The fluctuations in $\langle \bar{\psi}\psi \rangle$ are of the order of a few percent, while the averaged sign factor fluctuates almost by a factor of 2. The variation of $\langle \bar{\psi}\psi \rangle$ with mass μ_f is shown in Fig. 3. Once again, the statistical fluctuations are at most 3% for the whole range of masses from $\mu_f = 0.25$ to 1.5 (in units of inverse spatial lattice spacing). On the same figure, the values obtained from the analytic formula (16) are also indicated. In all cases the lattice is $5 \times 5 \times 80$. One sees that throughout

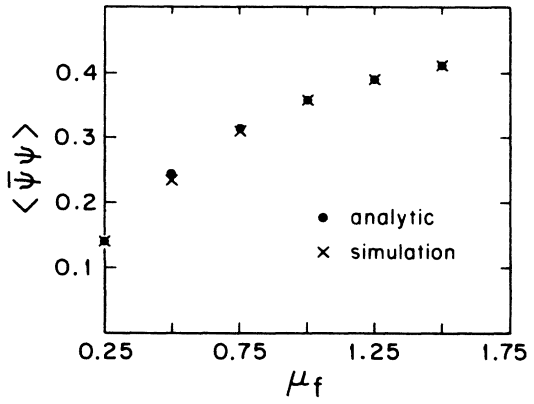

FIG. 3. Variation of $\langle \bar{\psi}\psi \rangle$ with μ_f.

the stated mass range the effect of finite temporal extent of the lattice is reduced to a few percent for a lattice with 80 time slices and a_0 chosen as indicated at the beginning of this section.

The important extensions of the procedure described here are (a) larger lattices, in particular in higher spatial dimensions, and (b) inclusion of interactions, e.g., with gauge fields. In the first case, one will need to go beyond the linear (i.e., $1 - a_0 H$) approximant to the fermionic transfer matrix. This should not be too difficult given the rather simple action of H on the spin variables. In the second, one will want to know the optimal update procedure (e.g., from the point of view of autocorrelation) in a system of interacting (bosonized) fermions and bosons. These matters are presently under investigation and will be discussed in a forthcoming publication.

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