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Monte Carlo calculations of coupled boson-fermion systems. I

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We present a formalism for carrying out Monte Carlo calculations of field theories with both boson and fermion degrees of freedom. The basic approach is to integrate out the fermion degrees of freedom and obtain an effective action for the boson fields to which standard Monte Carlo techniques can be applied. We study the structure of the effective action for a wide class of theories. We develop a procedure for making rapid calculations of the variation in the effective action due to local changes in the boson fields, which is essential for practical numerical calculations.

I. INTRODUCTION

Monte Carlo calculations have proven useful for studying a variety of field-theory problems in condensed-matter and high-energy physics. To date, virtually all such calculations have involved systems with boson degrees of freedom only; however, there has recently been considerable interest in extending Monte Carlo techniques to systems with interacting bosons and fermions.[1-5] In this paper we present the general formalism we have developed for carrying out such calculations. In a subsequent paper we shall give numerical results obtained from applying our formalism to a two-dimensional field theory.[6]

Our starting point is the path-integral formulation of field theory. The expectation value of an operator A is given by

$$\langle A\rangle = \int e^{-S}A \Big/ \int e^{-S}. \tag{1}$$

Here S is the Euclidean action, that is, the action defined at imaginary time, $\tau = it$. The integrals in Eq. (1) are over all possible configurations of the fields on which S and A depend.

The basic idea of a Monte Carlo calculation is to generate an ensemble of field configurations Σ_i, $i=1,\ldots,N$, such that the probability of a particular configuration Σ_j occurring is

$$e^{-S(\Sigma_j)} \Big/ \sum_{i=1}^{N} e^{-S(\Sigma_i)}.$$

Then

$$\langle A\rangle = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} A(\Sigma_i). \tag{2}$$

This approach can be applied directly only to pure boson systems. In the path-integral formulation of field theory fermions are represented by anticommuting c-number fields, so e^{-S} is not a c number and cannot serve as a relative probability.

In this paper we shall consider theories for which the continuum action can be written in the form

$$S = S_B + \int d\tau \int d^d x\, \psi^\dagger(x,\tau)\hat{O}\psi(x,\tau). \tag{3}$$

S_B is the pure boson action, $\psi(x,\tau)$ the fermion field, and d the number of space dimensions. $\hat{O}$ contains both derivative operators, mass terms, and the coupling of the fermions to the bosons. It is therefore a function of the boson fields. Theories with quartic fermion interactions can be written in the form of Eq. (3) through the introduction of auxiliary boson fields.

For theories of this type, the fermion degrees of freedom can be integrated out *ab initio*, leaving a pure boson theory to which one can apply standard Monte Carlo techniques.[1] However, difficult problems remain. In order to carry out the Monte Carlo calculation, one places the theory on a lattice in both space and imaginary time. New field configurations are generated by sweeping through the lattice and making a random change in the field variables on each lattice site or link. A particular change is accepted or rejected according to an algorithm which ensures that once equilibrium has been reached, the probability of a particular field configuration occurring is proportional to e^{-S}. For the Metropoulos algorithm,[7] of which we shall make use, it is necessary to compute the change in action corresponding to each field change. Local field theories without fermions are tractable because the calculation of the change in action due to the change in the field at a single site or link only requires knowledge of the fields in the immediate neighborhood of the change. The change in the action can be computed very rapidly for such theories.

For systems with interacting bosons and fermions with actions of the form given in Eq. (3),

the integration over the fermion degrees of freedom leaves a pure boson theory with an effective action defined by

$$e^{-S_{\text{eff}}} = e^{-S_B} \det\hat{O} . \tag{4}$$

S_B will in general be local, and therefore easy to deal with. However, the fermion determinant, $\det\hat{O}$, is inherently nonlocal, and repeated evaluations of its variations can be very time consuming. Since the reality and positivity of $\det\hat{O}$ is not guaranteed, the final form of our suggested effective action will be given latter, [Eq. (73)].

In Sec. II, we study the problem of integrating out the fermion degrees of freedom. We show that $\det\hat{O}$ can be reduced from the determinant of an operator that acts on both space and imaginary-time coordinates to the determinant of one that acts on space coordinates only. This reduction in dimensionality of the fermion determinant leads to a considerable savings of time in our numerical work.

In Sec. III, we introduce a lattice in both space and imaginary time. Our approach to putting the fermions on the lattice is designed to speed up the Monte Carlo calculations and to improve the convergence of the lattice theory to the continuum limit. It also avoids the doubling of the energy spectrum of the fermions encountered in some lattice theories.[8] We illustrate our lattice formulation by considering a solvable model in Sec. IV.

Finally, in Sec. V we present a detailed outline of our procedure for carrying out the Monte Carlo calculations.

II. FERMIONS IN A TIME-DEPENDENT EXTERNAL FIELD

In this section we study in detail the problem of performing the integration over the fermion degrees of freedom.

The fermion operator $\hat{O}$ defined in Eq. (3) can in general be written in the form[9]

$$\hat{O} = \frac{\partial}{\partial\tau} + H . \tag{5}$$

The single-particle "Hamiltonian," H, contains both space derivatives and couplings to the boson fields. For example, if we consider a system of nonrelativistic fermions coupled linearly to a boson field, $\varphi(x,\tau)$, then

$$H = -\nabla^2 + \omega + \lambda\varphi(x,\tau) . \tag{6}$$

The parameter ω sets the chemical potential. Relativistic fermions with the same scalar coupling would have

$$H = \frac{1}{i}\vec{\nabla}\cdot\vec{\alpha} + m\beta + \lambda\varphi(x,\tau)\beta , \tag{7}$$

where $\vec{\alpha}$ and β are the usual Dirac matrices.[8] Other types of couplings are, of course, possible and can be handled in the same general manner.

In practical numerical calculations, the range of both the space and imaginary-time variables must be finite. We impose periodic boundary conditions in the spatial directions for both fermion and boson fields. Restricting the imaginary-time to a finite range means that we are doing finite-temperature field theory. The expectation value defined in Eq. (1) is then a thermal average. We impose the restriction

$$0 \leq \tau \leq \beta \equiv 1/kT , \tag{8}$$

where T is the temperature. We of course recover the zero-temperature results when kT is much smaller than the other energy scales in the problem.

It is well known from finite-temperature statistical mechanics that boson Green's functions are periodic in imaginary time with period β, and fermion Green's functions are antiperiodic.[10] We must therefore require that a boson field, $\varphi(x,\tau)$, satisfy

$$\varphi(x,\tau+\beta) = \varphi(x,\tau) , \tag{9}$$

and that a fermion field, $\psi(x,\tau)$, satisfy

$$\psi(x,\tau+\beta) = -\psi(x,\tau) . \tag{10}$$

The "Hamiltonian," H, is of course periodic in τ.

We now return to the problem of performing the integration over the fermion fields. Substituting Eqs. (3) and (5) into Eq. (1), we see that if the operator A is independent of the fermion fields, then

$$\langle A\rangle = Z^{-1}\int e^{-S_B}\det\left(\frac{\partial}{\partial\tau}+H\right)A \tag{11}$$

with

$$Z = \int e^{-S_B}\det\left(\frac{\partial}{\partial\tau}+H\right) . \tag{12}$$

The integrals in Eqs. (11) and (12) are over all possible configurations of the boson fields.

The fermion Green's function is given by

$$\langle T[\Psi(x,\tau)\Psi^\dagger(x',\tau')]\rangle = Z^{-1}\int e^{-S_B}\det\left(\frac{\partial}{\partial\tau}+H\right)G(x,\tau;x',\tau') , \tag{13}$$

where $\Psi(x,\tau)$ is the second-quantized fermion field operator, T indicates the imaginary-time ordered product, and

$$G(x,\tau;x',\tau') = \left\langle x,\tau \left| \left(\frac{\partial}{\partial\tau}+H\right)^{-1} \right| x',\tau' \right\rangle$$
$$= \left[\det\left(\frac{\partial}{\partial\tau}+H\right)\right]^{-1} \int \delta\psi^\dagger\delta\psi \exp\left[-\int_0^\beta d\tau \int d^dx\, \psi^\dagger(x,\tau)\left(\frac{\partial}{\partial\tau}+H\right)\psi(x,\tau)\right] T[\psi(x,\tau)\psi^\dagger(x',\tau')]$$
$$\equiv \langle x|G(\tau,\tau')|x'\rangle . \tag{14}$$

More complicated fermion operators will clearly involve averages of products of G's.

Our next task is to obtain simplified expressions for det $(\partial/\partial\tau+H)$ and for the operator $G(\tau,\tau')$. Let us begin with the latter. It satisfies the differential equation

$$\left[\frac{\partial}{\partial\tau}+H(\tau)\right]G(\tau,\tau') = G(\tau,\tau')\left[\frac{\partial}{\partial\tau'}+H(\tau')\right]$$
$$= \delta(\tau-\tau')I , \tag{15}$$

where I is the identity operator. The boundary conditions are

$$G(\tau+\beta,\tau') = G(\tau,\tau'+\beta) = -G(\tau,\tau') . \tag{16}$$

In Eq. (15) H, G, and I are operators in coordinate space. The solution to Eqs. (15) and (16) can be written down by inspection. Defining

$$U(\tau,\tau') = T\exp\left(-\int_{\tau'}^{\tau} d\tau''H(\tau'')\right),$$

one finds that for $\beta>\tau>\tau'>0$

$$G(\tau,\tau') = U(\tau,\tau')J^{-1}(\tau')$$
$$= J^{-1}(\tau)U(\tau,\tau') , \tag{17}$$

while for $\beta>\tau'>\tau>0$

$$G(\tau,\tau') = -U(\tau,0)U(\beta,\tau')J^{-1}(\tau')$$
$$= -J^{-1}(\tau)U(\tau,0)U(\beta,\tau') \tag{18}$$

with

$$J(\tau) = I+U(\tau,0)U(\beta,\tau) . \tag{19}$$

For $\tau\neq\tau'$, Eqs. (17) and (18) satisfy Eq. (15) by definition of U and the time-ordered product. In addition

$$\lim_{\epsilon\to 0+}[G(\tau'+\epsilon,\tau') - G(\tau'-\epsilon,\tau')] = I , \tag{20}$$

so Eq. (15) is in fact satisfied for all values of τ and τ'.

Equations (17) and (18) are straightforward generalizations of formulas which are well known when H is independent of τ. In that case we can introduce eigenfunctions and eigenvalues of H satisfying

$$H|\chi_k\rangle = \epsilon_k|\chi_k\rangle \tag{21}$$

and rewrite Eq. (17) in the familiar form

$$G(\tau,\tau') = e^{-(\tau-\tau')H}(I+e^{-\beta H})^{-1}$$
$$= \sum_k e^{-(\tau-\tau')\epsilon_k}(1+e^{-\beta\epsilon_k})^{-1}|\chi_k\rangle\langle\chi_k| , \tag{22}$$

and Eq. (18) as

$$G(\tau,\tau') = -e^{-[\beta-(\tau-\tau')]H}(I+e^{-\beta H})^{-1}$$
$$= -\sum_k e^{-[\beta-(\tau'-\tau)]\epsilon_k}(1+e^{-\beta\epsilon_k})^{-1}|\chi_k\rangle\langle\chi_k| . \tag{23}$$

We now turn our attention to simplifying the fermion determinant. It is convenient to make the substitution $H\to\eta H$, where η is a constant, and write

$$D(\eta) = \det_{x,\tau}\left(\frac{\partial}{\partial\tau}+\eta H\right)$$
$$= \int \delta\psi^\dagger\delta\psi \exp\left[-\int_0^\beta d\tau \int d^dx\, \psi^\dagger(x,\tau) \times\left(\frac{\partial}{\partial\tau}+\eta H\right)\psi(x,\tau)\right] . \tag{24}$$

We wish to show that $D(\eta)$ is equal to

$$\bar{D}(\eta) = \det_x\left[I+T\exp\left(-\int_0^\beta d\tau\,\eta H(\tau)\right)\right], \tag{25}$$

up to an overall constant factor. The subscripts on det in Eqs. (24) and (25) are to remind us that in Eq. (24) we are taking the determinant of an operator that acts on functions of x and τ, while in Eq. (25) we are taking the determinant of one which acts on functions of x only.

Let us differentiate Eqs. (24) and (25) with respect to η. From Eq. (25) we obtain

$$\frac{d}{d\eta}\ln\bar{D}(\eta) = \int_0^\beta d\tau\,\mathrm{tr}_x[H(\tau)G_\eta(\tau-\epsilon,\tau)]$$
$$= \int_0^\beta d\tau \int d^dx\, H(\tau)G_\eta(x,\tau-\epsilon,x',\tau)\Big|_{x=x'} , \tag{26}$$

where the Green's function G_η is given by Eqs. (14), (17), and (18) with H replaced by ηH.

On the other hand, Eq. (24) gives

$$\frac{d}{d\eta}\ln D(\eta) = -D(\eta)^{-1}\int_0^\beta d\tau \int d^dx \int \delta\psi^\dagger\delta\psi \exp\left[-\int_0^\beta d\tau' \int d^dx' \psi^\dagger(x',\tau')\left(\frac{d}{d\tau'}+\eta H\right)\psi(x',\tau')\right]\psi^\dagger(x,\tau)H(\tau)\psi(x,\tau)\,. \tag{27}$$

As can be seen from Eq. (20), Eq. (27) is not well defined until we introduce a prescription for the product of the two fermion fields with equal time arguments in the action. Soper has shown that if the original second-quantized Hamiltonian is normal ordered, the correct prescription is to replace $\psi(x,\tau)$ in the action by $\lim_{\epsilon\to 0+}\psi(x,\tau-\epsilon)$.[9]

Making use of Eqs. (18) and (27), we see that with this prescription

$$\frac{d}{d\eta}\ln D(\eta) = \frac{d}{d\eta}\ln \bar{D}(\eta)\,. \tag{28}$$

As a result, up to an overall constant, which can be set equal to one by a suitable choice of the measure of the functional integral over ψ and ψ^*,

$$D = \det{}_{x,\tau}\left(\frac{\partial}{\partial\tau}+H\right) = \det{}_x\left[I+T\exp\left(-\int_0^\beta d\tau\, H(\tau)\right)\right], \tag{29}$$

which is the desired result.

For H independent of τ, D is the partition function for a system of fermions which interact with a time-independent external field, but not with each other. In this case

$$D = \det{}_x(I+e^{-\beta H}) = \prod_k (1+e^{-\beta\epsilon_k})\,, \tag{30}$$

which is the standard result. Notice that our limiting prescription for defining the action was essential to obtain this result. For example, had we replaced $\psi(x,\tau)$ in the action by $\lim_{\epsilon\to 0+}\psi(x,\tau+\epsilon)$, then we would have obtained Eq. (29) with $T\exp[-\int_0^\beta d\tau\, H(\tau)]$ replaced by $A\exp[\int_0^\beta d\tau\, H(\tau)]$, where A is the anti-time ordering operator. In this case Eq. (30) would have $e^{-\beta H}$ and $e^{-\beta\epsilon_k}$ replaced by $e^{\beta H}$ and $e^{\beta\epsilon_k}$, respectively.

III. FERMIONS ON A LATTICE

In order to carry out the Monte Carlo calculations we must put the theory on a lattice in both space and imaginary time. The pure boson action, S_B, is treated in the standard way. That is, the spacetime continuum is divided into cubes and each cube is replaced by a lattice point. Matter fields are defined on the lattice points, and their derivatives in the continuum theory go over into finite differences on the lattice. Gauge fields are defined on the links between lattice points.

Some care must be taken in transferring fermion operators such as

$$U(\tau,\tau') = T\exp\left(-\int_{\tau'}^{\tau} d\tau'' H(\tau'')\right) \tag{31}$$

to the lattice. If we first introduce a spatial lattice with N points in each space direction, then $H(\tau)$ becomes an $N^d\times N^d$ matrix. Let us now imagine dividing the time interval $0\le\tau\le\beta$ into L segments of width $\Delta\tau$, and write

$$U(\tau,\tau') = U(\tau,\tau-\Delta\tau)U(\tau-\Delta\tau,\tau-2\Delta\tau)\cdots U(\tau'+\Delta\tau,\tau')\,. \tag{32}$$

If we concentrate on the interval $(m-1)\Delta\tau\le\tau\le m\Delta\tau$ we can expand $H(\tau)$ in a Taylor series

$$H(\tau) = H_m + [\tau-(m-\tfrac{1}{2})\Delta\tau]H'_m+\cdots\,, \tag{33}$$

where H_m and H'_m are, respectively, $H(\tau)$ and its first derivative evaluated at the point $\tau=(m-\frac{1}{2})\Delta\tau$. Substituting Eq. (33) into Eq. (31), we see that

$$U_m \equiv U(m\Delta\tau,(m-1)\Delta\tau) = \exp[-\Delta\tau H_m + O(\Delta\tau^3)]\,. \tag{34}$$

At first glance it might seem that within the spirit of the lattice approximation we could expand the right-hand side of Eq. (34) and take $U_m \simeq I-\Delta\tau H_m$. We do not choose to do so for a number of reasons. In any practical calculation $\Delta\tau$ must be kept finite, while the eigenvalues of the H_m can be large. This means that Eq. (34) can lead to good agreement with the continuum results even when the linear approximation fails badly. To illustrate this point, consider the case in which the H_m are independent of m. Using Eq. (34) for U_m, we obtain exactly the same result for the fermion determinant as was obtained in Eq. (30) from the continuum theory. On the other hand, if we approximate U_m by $I-\Delta\tau H$, we find

$$D \simeq \det[I+(I-\Delta\tau H)^m] = \prod_k\left[1+\exp\left(\frac{\beta}{\Delta\tau}\ln(1-\Delta\tau\epsilon_k)\right)\right]. \tag{35}$$

Although Eq. (35) does reduce to Eq. (30) in the limit $\Delta\tau\to 0$, the convergence is slow. Clearly for $\epsilon_k \gtrsim 1/\Delta\tau$, Eq. (35) is unphysical. Finally, we shall see in the next section that if one approximates U_m by $1-\Delta\tau H_m$, the limit $\Delta\tau\to 0$ does not in general commute with the integration over the boson degrees of freedom. Note that during this integration H_m can achieve a large value, and $\Delta\tau H_m$ is not always small.

We can make one further simplification of Eq. (34). We write H_m as the sum of a "kinetic energy" matrix, K, which is diagonal in momentum space,

and a "potential energy" matrix, V_m, which is diagonal in coordinate space.[8,11] For example, for H given by Eq. (6) we take

$$K=-\nabla^2+\omega\,, \tag{36}$$

where ∇^2 is the lattice Laplacian. Denoting by $\varphi_m(i)$ the field variable at lattice spatial coordinate i and time $\tau_m=(m-\frac{1}{2})\Delta\tau$, the potential V_m for this model has matrix elements

$$V_m(i,i')=\delta_{i,i'}\lambda\varphi_m(i)\,. \tag{37}$$

Irrespective of the form of K and V_m we can rewrite Eq. (34) in the form

$$U_m\simeq e^{-\Delta\tau K/2}e^{-\Delta\tau V_m}e^{-\Delta\tau K/2}\,, \tag{38}$$

where we have again retained terms up to order $\Delta\tau^3$.

Using Eq. (38) the lattice form of the fermion determinant can be written as

$$D=\det(I+B_L B_{L-1}\cdots B_1)\,, \tag{39}$$

where

$$B_m=e^{-\Delta\tau K}e^{-\Delta\tau V_m}\,. \tag{40}$$

The lattice version of Eqs. (17)–(19) for the time evolution operator can also be written down in terms of the B_m. For example, for $\tau=(m-\frac{1}{2})\Delta\tau > \tau'=(m'-\frac{1}{2})\Delta\tau$

$$G(\tau,\tau')=e^{\Delta\tau K/2}B_m\cdots B_{m'+1}[I+B_{m'}\cdots B_1 B_L\cdots B_{m'-1}]^{-1}e^{-\Delta\tau K/2}\,. \tag{41}$$

Since the operator $e^{-\Delta\tau K}$ is diagonal in momentum space, it can be simply written down in terms of its eigenvalues. As a result, the doubling of the energy spectrum found in some lattice formulations can be avoided even for relativistic fermions.

We conclude this section by writing down the fermion action we would have obtained had we gone onto the lattice before integrating out the fermion fields. Now the requisite equations of motion using Eqs. (34) and (38) are

$$\begin{aligned}\psi_m-\psi_{m-1}&=-(1-U_m)\psi_{m-1}\\&\equiv-\Delta\tau H_m^{\rm eff}\psi_{m-1}\,,\end{aligned} \tag{42}$$

where the effective Hamiltonian is given by

$$\begin{aligned}\Delta\tau H_m^{\rm eff}&=I-e^{-\Delta\tau H_m}\\&\simeq e^{\Delta\tau K/2}(I-e^{-\Delta\tau K}e^{-V_m})e^{-\Delta\tau K/2}\end{aligned} \tag{43}$$

with errors of order $(\Delta\tau)^3$. Using the latter form and absorbing a factor of $\exp(-\frac{1}{2}\Delta\tau K)$ into ψ_m and $\exp(\frac{1}{2}\Delta\tau K)$ into $\psi_m^\dagger$, the lattice form of the action, Eq. (3), becomes

$$S=S_B+(\Delta x)^d\sum_{\substack{m,m'\\ i,i'}}\psi_m^\dagger(i)\hat{O}_{m,m'}(i,i')\psi_{m'}(i') \tag{44}$$

with

$$\hat{O}=\begin{bmatrix} I & 0 & 0 & \cdots & B_1\\ -B_2 & I & 0 & \cdots & 0\\ 0 & -B_3 & I & \cdots & 0\\ \cdot & \cdot & \cdot & & \cdot\\ \cdot & \cdot & \cdot & & \cdot\\ \cdot & \cdot & \cdot & & \cdot\\ & & & I & 0\\ 0 & 0 & 0 & -B_L & I \end{bmatrix}\,. \tag{45}$$

Recall that I and B_m are themselves $N^d\times N^d$ matrices.

The interested reader will easily verify that

$$\begin{aligned}&\det\hat{O}=D=\det(I+B_L\cdots B_1)\,,\\ &\hat{O}^{-1}_{m,m'}=\begin{cases}B_m B_{m-1}\cdots B_{m'+1}(I+B_{m'}\cdots B_1 B_L\cdots B_{m'-1})^{-1}\,, & m\geq m'\\ -B_m\cdots B_1 B_L\cdots B_{m'+1}(I+B_{m'}\cdots B_1 B_L\cdots B_{m'-1})^{-1}\,, & m<m'\,.\end{cases}\end{aligned} \tag{46}$$

Notice that O^{-1} differs from the Green's function G of Eq. (41) by a factor of $e^{\Delta\tau K/2}$ on the left and a factor $e^{-\Delta\tau K/2}$ on the right. When we take data in the Monte Carlo calculation we average over all points with the same space and time separations. The reader can easily verify that with this procedure the average values of matrix elements of G and O^{-1} are identical.

In the limit $\Delta\tau\to 0$ we can take $B_m\simeq I-\Delta\tau H_m$, and Eq. (41) then becomes

$$\begin{aligned}S=S_B&=\Delta\tau(\Delta x)^d\sum_m[\psi_m^\dagger(\psi_m-\psi_{m-1})/\Delta\tau+\psi_m^\dagger H_m\psi_{m-1}]\\&\equiv S_B+\int_0^\beta d\tau\int d^dx\psi^\dagger\left(\frac{\partial}{\partial\tau}+H\right)\psi\,,\end{aligned} \tag{47}$$

which is the result of Soper.[9] Notice that we automatically obtain an asymmetric lattice definition of $\partial/\partial\tau$. Had we used the symmetric lattice derivative defined by $[(\partial/\partial\tau)\psi]_m=(\psi_{m+1}-\psi_{m-1})/2\Delta\tau$, we would have had the usual spectrum doubling prob-

lems, and that in turn would have led to incorrect results for the fermion Green's functions.

IV. A SOLVABLE MODEL

In this section we illustrate and test our ideas by considering the quantum-mechanics model of a single fermion interacting with a boson. The continuum action is

$$S=\int_0^\beta d\tau\left[\frac{1}{2}\left(\frac{\partial\varphi}{\partial\tau}\right)^2+\tfrac{1}{2}\Omega^2\varphi^2 + \psi^\dagger\left(\frac{\partial}{\partial\tau}+\omega+\lambda\varphi\right)\psi\right]. \tag{48}$$

This model is most easily solved in the second-quantized formalism. The Hamiltonian is

$$\tilde{H}=\Omega b^\dagger b+\omega c^\dagger c+(2\Omega)^{-1/2}\lambda(b^\dagger+b)c^\dagger c\,, \tag{49}$$

where b and c are, respectively, the boson and fermions destruction operators. With a little algebra we find

$$\begin{aligned} Z&=\mathrm{tr}e^{-\beta\tilde{H}}=(1+e^{-\beta\bar{\omega}})/(1-e^{-\beta\Omega})\,,\\ \langle\varphi\rangle&=Z^{-1}\,\mathrm{tr}[e^{-\beta\tilde{H}}(b^\dagger+b)/(2\Omega)^{1/2}]\\ &=-(\lambda/\Omega^2)(1+e^{\beta\bar{\omega}})^{-1}\,, \end{aligned} \tag{50}$$

and

$$\begin{aligned} \langle G\rangle&=Z^{-1}\,\mathrm{tr}[e^{-\beta\tilde{H}}c(\tau)c^\dagger(0)]\\ &=\exp\{-\tau\bar{\omega}+\tfrac{1}{2}(\lambda^2/\Omega^3)(1-e^{-\beta\Omega})^{-1}\\ &\quad\times[e^{-\beta\Omega}(e^{\tau\Omega}-1)+e^{-\tau\Omega}-1)]\}\\ &\quad\times(1+e^{-\beta\bar{\omega}})^{-1}\,, \end{aligned} \tag{51}$$

where

$$c(\tau)=e^{\tau H}ce^{-\tau H} \tag{52}$$

and

$$\bar{\omega}=\omega-\tfrac{1}{2}(\lambda^2/\Omega^2)\,. \tag{53}$$

Let us now go onto the lattice. The action can then be written in the form

$$S=\sum_{m,m'=1}^{L}(\varphi_m P_{m,m'}\varphi_{m'}+\psi_m^\dagger\hat{O}_{m,m'}\psi_{m'})\,. \tag{54}$$

The matrix O is given by Eq. (43), but the B_m are numbers in this simple model rather than matrices

$$B_m=e^{-\Delta\tau(\omega+\lambda\varphi_m)}\,. \tag{55}$$

The fermion determinant is

$$D=\det\hat{O}=1+e^{-\beta\omega}\exp\left(-\Delta\tau\lambda\sum_{m=1}^{L}\varphi_m\right). \tag{56}$$

Notice that D is positive definite, but would not be if we had approximated B_m by $I-\Delta\tau H_m$.

The matrix P is defined by

$$\sum_{m,m'=1}^{L}\varphi_m P_{m,m'}\varphi_{m'}=\sum_{m=1}^{L}[(P_+^2+P_-^2)\varphi_m^2-2P_+P_-\varphi_m\varphi_{m-1}] \tag{57}$$

with $\varphi_0\equiv\varphi_m$ and

$$\begin{aligned} P_+&=(2\Delta\tau)^{-1/2}e^{\Delta\tau\Omega/2}\,,\\ P_-&=(2\Delta\tau)^{-1/2}e^{-\Delta\tau\Omega/2}\,. \end{aligned} \tag{58}$$

In the limit $\Delta\tau\Omega\ll1$, Eq. (60) reduces to

$$\sum_{m,m'=1}^{L}\varphi_m P_{m,m'}\varphi_{m'}\simeq\sum_{m=1}^{L}\left[\frac{1}{2\Delta\tau}(\varphi_m-\varphi_{m-1})^2+\tfrac{1}{2}\Delta\tau\Omega^2\varphi_m^2\right]. \tag{59}$$

We have chosen this somewhat unconventional form for P in order that the boson correlation functions reduce to the continuum ones for $\lambda=0$ and $\Delta\tau$ finite.

The lattice partition function Z_L is given by

$$Z_L=\int_{-\infty}^{\infty}\prod_{m=1}^{L}\frac{d\varphi_m}{(2\pi\Delta\tau)^{1/2}}e^{-\Delta\tau\vec{\varphi}\cdot P\cdot\vec{\varphi}}(1+e^{-\beta\omega}e^{-\Delta\tau\lambda\vec{\varphi}\cdot\vec{n}})\,, \tag{60}$$

where we have introduced the vector notation $\vec{\varphi}=(\varphi_1,\ldots,\varphi_L)$, $\vec{n}=(1,1,\ldots,1)$. The integrations in Eq. (60) are easily done and we obtain

$$\begin{aligned} Z_L&=[(2\Delta\tau)^L\det P]^{-1/2}(1+e^{-\beta\omega}e^{-\Delta\tau\lambda^2\vec{n}\cdot P^{-1}\cdot\vec{n}/4})\\ &=(1+e^{-\beta\bar{\omega}'})/(e^{\beta\Omega/2}-e^{-\beta\Omega/2}) \end{aligned} \tag{61}$$

with

$$\bar{\omega}'=\omega-\tfrac{1}{2}\lambda^2/\Omega'^2 \tag{62}$$

and

$$\Omega'=\sinh(\tfrac{1}{2}\Delta\tau\Omega)/\tfrac{1}{2}\Delta\tau\,.$$

Apart from an overall factor of $e^{-\beta\Omega/2}$, which arises from the zero-point energy of the boson, and the replacement $\bar{\omega}\to\bar{\omega}'$, Eq. (61) is identical to Eq. (49).

Notice that if we had approximated B_m by $I-\Delta\tau H_m$, performed the functional integration over φ, and then taken the limit $\Delta\tau\to0$, we would have found that in Eq. (61) the quantity $\vec{n}\cdot P^{-1}\cdot\vec{n}$ was replaced by $\vec{n}\cdot P^{-1}\cdot\vec{n}-\mathrm{tr}P^{-1}$. In other words, we would *not* have obtained the correct continuum limit. The difficulty can most easily be seen by making a Fourier expansion of the boson field. We then see that the $(\partial\varphi/\partial\tau)^2$ term in the boson action damps all modes except the zero-frequency one when their amplitudes are of order $(\Delta\tau)^{1/2}$. However, the zero-frequency mode is not damped until its amplitude is of order $(\Delta\tau)^{-1/2}$. As a result, when expanding D in powers of $\Delta\tau\varphi_m$, we cannot drop terms of order $(\Delta\tau\varphi_m)^2$, if we expect to recover the continuum limit. This result is ex-

pected to hold in general.

Proceeding as above we find that

$$\langle \varphi_m \rangle = -(\lambda/\Omega')(1+e^{\beta\bar{\omega}'})^{-1} \tag{63}$$

and

$$\begin{aligned}\langle G(\tau)\rangle &= \langle \psi_m \psi_1^\dagger \rangle \\ &= \exp\{-\tau\bar{\omega}' + \tfrac{1}{2}(\lambda^2/\Omega'^2\Omega'')(1-e^{-\beta\Omega})^{-1} \\ &\quad \times [e^{-\beta\Omega}(e^{\tau\Omega}-1)+(e^{-\tau\Omega}-1)]\} \\ &\quad \times (1+e^{-\beta\bar{\omega}'})^{-1}\end{aligned} \tag{64}$$

where $\tau = (m-\frac{1}{2})\Delta\tau$ and $\Omega'' = \sinh(\Delta\tau\Omega)/\Delta\tau$. Again our results are identical with the continuum ones except for some replacements of Ω by Ω' and Ω''. Convergence to the continuum limit is rapid for $\Delta\tau\Omega < 1$ and does not require that $\Delta\tau\omega$ be small.

V. MONTE CARLO CALCULATIONS

We are now in a position to describe our procedure for performing Monte Carlo calculations.

We start by specifying an initial field configuration. Generally we either choose the field to be constant or we assign a random value to it on each lattice site. Next we bring the system into equilibrium so that the probability of a particular field configuration, Σ_j, occurring is proportional to $e^{-S_{\text{eff}}(\Sigma_j)}$, where S_{eff} will be fully defined shortly. To do this we pass through the lattice a number of times. At each site we make a random change in the field and calculate the corresponding change in the effective action, ΔS_{eff}. We accept or reject a particular field change according to the Metropoulos algorithm[7] which prescribes that the change should always be accepted if $\Delta S_{\text{eff}} \leq 0$ and should be accepted with probability $e^{-\Delta S_{\text{eff}}}$ if $\Delta S_{\text{eff}} > 0$.

Once the system has reached equilibrium we calculated the average value of operators of interest by collecting data for a large number of statistically independent field configurations. To ensure that the field configurations are independent, we must pass through the lattice a number of times between collecting data and updating the field in the manner just described.

The calculation of the change in the effective action is by far the most time-consuming operation we have to carry out. As was pointed out in the Introduction, the change in the boson action, S_B, can be obtained rapidly for local field theories. The difficult problem is to calculate the change in the fermion determinant rapidly.

Let us consider the updating of the fermion determinant in detail. We assume that the matrix V_m is diagonal[11] and that the change in the boson fields at a single lattice point leads to a change in a single element of V_m. More general forms for V_m can be treated with a slight additional complication as is discussed in Ref. 2.

We assume that a change in the field element $\varphi_m(i) \to \varphi_m(i) + \delta\varphi_m(i)$ induces a change $V_m(i) \equiv V_m(i,i) \to V_m(i) + \delta V_m(i)$, with all other elements of V_m (and V_n, $n \neq m$) remaining fixed. We then have $B_m \to B_m \Delta_m$ where Δ_m is a diagonal matrix with

$$\begin{aligned}&\Delta_m(i,i) = e^{-\Delta\tau\delta V_m(i)} \equiv N_m(i) + 1\,, \\ &\Delta_m(j,j) = 1\,, \quad j \neq i\,.\end{aligned} \tag{65}$$

To compute the change in the effective action, we need the ratio R of the fermion determinants before and after the field change. Since Eq. (39) can be rewritten in the form

$$D = \det(I + B_{m-1}B_{m-2}\cdots B_1 B_L \cdots B_m)\,, \tag{66}$$

we have[12]

$$\begin{aligned}R &= \frac{\det(I + B_{m-1}\cdots B_1 B_L \cdots B_m \Delta_m)}{\det(I + B_{m-1}\cdots B_1 B_L \cdots B_m)} \\ &= \det[I + (I - g_m)(\Delta_m - I)] \\ &= 1 + [1 - g_m(i,i)]N_m(i)\,,\end{aligned} \tag{67}$$

where

$$g_m = (I + B_{m-1}\cdots B_1 B_L \cdots B_m)^{-1}\,. \tag{68}$$

Thus it is trivial to compute the ratio of determinants provided the Green's function g_m is known. Suppose we do know it and that we accept field change $\varphi_m(i) \to \varphi_m(i) + \delta\varphi_m(i)$. We can then compute the updated Green's function, $\bar{g}_m$, from the relation

$$\begin{aligned}\bar{g}_m &= (I + B_{m-1}\cdots B_1 B_L \cdots B_m \Delta_m)^{-1} \\ &= g_m - (I - g_m)(\Delta_m - I)\bar{g}_m\,,\end{aligned} \tag{69}$$

which can be trivially solved to give[12]

$$\bar{g}_m(j,k) = g_m(j,k) - \frac{[\delta_{ji} - g_m(j,i)]N_m(i)g_m(i,k)}{1 - [1 - g_m(i,i)]N_m(i)}\,. \tag{70}$$

After we have updated the field at every spatial point in the time slice $\tau_m = (m-\frac{1}{2})\Delta\tau$, we can go on to the next time slice by making use of Eq. (66) with m replaced by $m+1$, and the relation

$$\begin{aligned}g_{m+1} &= (I + B_m \cdots B_1 B_L \cdots B_{m+1})^{-1} \\ &= B_m g_m B_m^{-1}\,.\end{aligned} \tag{71}$$

Our strategy should now be clear. At the beginning of the calculation we obtain g_1 either by choosing the starting field configuration to be trivial [i.e., by taking $\varphi_m(i)$ to be independent of m and i] or by taking the time to compute it numerically once. We then sweep through the lattice one time slice at a time. In order to decide whether to accept a particular field change we need only calculate the ratio of determinants via Eq. (67). The lengthier process of updating g_m must be per-

formed only when we accept a field change which happens roughly 50% of the time in our numerical calculations.

Notice that if there are N lattice points in each of the d spatial directions, the updating of g_m requires N^{2d} steps. This should be compared to the approximately N^{3d} steps required to make a direct calculation of the fermion determinant. Of course a direct calculation of $\det(\partial/\partial\tau + H)$ without eliminating the time coordinate would have required approximately M^3N^{3d} steps.

Up to now we have tacitly assumed that the fermion determinant is positive definite, but this is not necessarily the case. Each of the B_m matrices is a product of two positive-definite Hermitian matrices. However, products of such matrices need not be positive definite, so D need not be positive for each individual field configuration. We do believe that D will be positive for those field configurations that dominate the functional integrals, and in the calculations we have done to date D does not change sign.

The quantity $1 - g_m(i,i)$ is the probability of a fermion being at the point i at the time τ_m, so its expectation value must lie in the range zero to one. From Eq. (65) we see that $-1 < N_m(i) < \infty$, so we learn from Eq. (67) that D can change sign only if $g_m(i,i)$ takes on an unphysical value.

For field configurations which vary slowly enough in time so that the adiabatic approximation can be used in computing the B_m product, the fermion determinant simplifies to

$$D = \prod_k \left[1 + \exp\left(-\Delta\tau \sum_{m=1}^{L} \epsilon_m(k)\right)\right], \tag{72}$$

where $\epsilon_m(k)$ is the kth eigenvalue of H_m. Although the adiabatic approximation is not valid in general, Eq. (72) does illustrate the fact that D could only become negative when the boson fields vary rapidly in time, and such field configurations are ordinarily damped by time derivatives in the boson action S_B.

To perform a Monte Carlo integration over a real function $F(\Sigma_j)$, the optimum probability distribution for the random configurations, Σ_j, is just $F(\Sigma_j)$ itself if F is real and never negative. However, if F does change sign, then it is simple to show that the probability distribution that yields the minimum dispersion is $|F(\Sigma_j)|$. Since it is conceivable that D can become negative (and even complex as we shall see) we advocate performing the Monte Carlo calculations with the effective action defined by

$$e^{-S_{\text{eff}}} = e^{-S_B}|\mathrm{Re}D| . \tag{73}$$

If we denote the expectation value of an operator, A, with respect to this effective action by $\langle A\rangle_{ABS}$, then the expectation values of physical interest defined in Eq. (1) are given by

$$\langle A\rangle = \langle AD/|\mathrm{Re}D|\rangle_{ABS}/\langle D/|\mathrm{Re}D|\rangle_{ABS} . \tag{74}$$

This approach will be useful and convergent provided there are not important cancellations between regions of function space in which D has opposite signs, and we have just argued that this will not be the case.

Up to now we have assumed that H is real as well as Hermitian. If this is not the case, then it is possible for D to become complex for particular field configurations. However, in such cases there will always be a symmetry operation on the boson fields that will leave S_B invariant but take H into H^*. As a result, in such theories it is possible to replace D by ReD and proceed as outlined above.

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