Efficient algorithm for numerical simulations of the fermion-scalar systems

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An efficient algorithm is proposed for computer simulations of the lattice fermion-scalar models. Comparisons with the results from the hybrid Monte Carlo (HMC) method for a fermion-gauge-scalar model are made, and the HMC data are well reproduced. The advantage of our algorithm, in addition to its accessibility to the chiral limit, is its lower computational costs for different bare parameters, therefore, it is very suitable for analyzing the phase structure.

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I. INTRODUCTION

The lattice simulations of the fermion-scalar models have attracted interest because they can provide information on the nonperturbative aspects of the standard model and beyond. The main activities have focused on the following areas.

(a) The Higgs model at finite temperature. The properties of electroweak phase transition might be relevant for the development of the early Universe and baryogenesis. Up to now, only quenched simulations have been carried out. The fermions should finally be included since they would play an important role at finite temperature.

(b) Upper bound for the Higgs and fermion masses from the Yukawa models.

(c) More recently, it has been argued that some fermion-gauge-scalar models with a dynamical chiral broken phase at strong gauge coupling and chiral phase transition induced by the scalar field might be considered as a possible alternative to the Higgs mechanism, as discussed in [1].

The simulation of quantum field theory with fermions is an extremely demanding task. Furthermore, it might be expensive for the conventional algorithms to directly approach the chiral limit, i.e., the most interesting case of the models (a) and (c). For the gauge-fermion systems, an algorithm [2–4] has been developed for tackling this problem. The purpose of this work is to extend this algorithm to the fermion-gauge-scalar or fermion-scalar systems.

The rest of the paper is organized as follows. Section II describes our new algorithm. The saddle-point analysis is made in Sec. III. In Sec. IV, the numerical results are described and the hybrid Monte Carlo (HMC) method is used[1] to test against the algorithm. Conclusions are summarized in Sec. V with some discussions about the possible extension to the Yukawa models.

II. THE ALGORITHM

Let me first discuss the fermion-gauge-scalar models described by

$$S = -6V\beta S_p(U) - 8V\kappa S_l(U,\phi) + S_f(U,\psi) \qquad (2.1)$$

with

$$S_p(U) = \frac{1}{6V}\sum_p \mathrm{Re}(U_p),$$

$$S_l(U,\phi) = \frac{1}{4V}\sum_{x,\mu} \mathrm{Re}(\phi_x^\dagger U_{x,\mu}\phi_{x+\mu}),$$

$$S_f(U,\psi) = \bar{\psi}\Delta(U)\psi,$$

$$\Delta(U) = \not{p}^{\mathrm{latt}}(U) + m, \qquad (2.2)$$

where V is the lattice volume, β is related to the bare gauge coupling, U_p is the product of gauge link variables, $U_{x,\mu} = e^{igaA_{x,\mu}}$ around the elementary plaquette, κ is the hoping parameter, ϕ and ψ are, respectively, the scalar and fermion fields, and $\Delta(U)$ the fermionic matrix, with m the fermion mass and $\not{p}^{\mathrm{latt}}$ the massless Dirac operator on the lattice. Without loss of generality, the scalar modulus is fixed.

A standard prescription is to integrate out the fermionic degrees of freedom, so that the partition function becomes

$$Z = \int [dU][d\phi][d\phi^\dagger] \exp[6V\beta S_p(U) + 8V\kappa S_l(U,\phi)] \times [\det\Delta(U)]^{N_f^{\mathrm{latt}}}, \qquad (2.3)$$

where $\det\Delta(U)$ is the fermionic determinant and N_f^{latt} is the number of flavors taking into account the species doubling. The effects of dynamical fermions come from $\det\Delta(U)$, which numerical evaluation requires in general a huge CPU time due to nonlocality and dependence on the configurations for different bare parameters m, β, κ, and N_f. Nonlocality implies that small fluctuations in U would lead to large fluctuations in $\det\Delta(U)$, and

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[1]This part was done in collaboration with W. Franzki, C. Frick, and J. Jersák.

therefore prohibit local algorithms such as the Metropolis method. The HMC method has been accepted as the most efficient one for dynamical fermions.

Here we present a different and efficient algorithm for the fermion-gauge-scalar systems, which is applicable to arbitrary fermion masses, possibly including the chiral limit. The microcanonical fermionic average (MFA) method proposed in [2–4], and tested in the Schwinger model [5], has been shown to be useful for the phase structure analysis of the gauge-fermion systems, in particular for the ground-state properties in the chiral limit. Our algorithm to be discussed here is a delicate extension of the MFA method to the fermion-gauge-scalar systems. The essential idea of the algorithm is the computation of the full effective action as a function of the pure gauge energy E_p and other bare parameters such as m, N_f, β, and κ, using the microcanonical average process. Such a process would lead to significant reduction of the fluctuations in $\det\Delta(U)$.

What is new in our algorithm with respect to the MFA method is the treatment of the scalar field. A central question now is how to define the effective fermionic action. We hope it does not depend on at least some bare coupling parameter but depends on its corresponding energy so that it is not necessary to repeat the simulations of the effective fermionic action at different values of this bare parameter, fermion mass, and flavor number. In [2–4] it has been shown how this is realized in the fermion-gauge models. In the models described by (2.2), it also seems possible to perform the microcanonical updates for the gauge configurations U by fixing the gauge energy E_p, i.e., by inserting the identity

$$\int dE_p \delta[S_p(U) - E_p] \exp(6V\beta E_p) = \exp[6V\beta S_p(U)] \tag{2.4}$$

into the partition function (2.3). The result is

$$Z = \int dE_p \exp(6\beta V E_p) \int [dU][d\phi][d\phi^\dagger] \delta[S_p(U) - E_p] \times \exp[8V\kappa S_l(U,\phi)][\det\Delta(U)]^{N_f^{\text{latt}}}. \tag{2.5}$$

Can the link energy E_l and hopping parameter κ be factorized out of the integral $\int [dU][d\phi][d\phi^\dagger]$ in a way similar to that for the gauge energy? The answer is no. The reason is that $S_l(U,\phi)$ can neither be simultaneously fixed during the updates nor be expressed as a function of E_p. We solve this problem by introducing the density of states

$$M(E_p,\kappa) = \int [dU][d\phi][d\phi^\dagger] \delta[S_p(U) - E_p] \times \exp[8V\kappa S_l(U,\phi)], \tag{2.6}$$

and defining the effective fermionic action $S_{\text{eff}}^F(E_p, m, N_f, \kappa)$ by

$$\exp[-S_{\text{eff}}^F(E_p,m,N_f,\kappa)] = \langle [\det\Delta(U)]^{N_f^{\text{latt}}} \rangle_{E_p} = \frac{\int [dU][d\phi][d\phi^\dagger] \delta[S_p(U) - E_p] \exp[8V\kappa S_l(U)][\det\Delta(U)]^{N_f^{\text{latt}}}}{M(E_p,\kappa)}, \tag{2.7}$$

where the fermionic determinant of configuration U is related to m and the positive eigenvalues $\lambda_i(U)$ of $\not{D}^{\text{latt}}(U)$ by

$$\det\Delta(U,m) = \prod_{i=1}^{V/2} [\lambda_i^2(U) + m^2]. \tag{2.8}$$

Equations (2.6) and (2.7) contain some new ideas of this paper with respect to those in MFA [2–4]. The introduction of the "effective scalar action," which is generally a function of E_p and κ, and requires some extra complicated computations [4], is completely avoided. The effects of the scalar field are absorbed into the density of states and effective fermionic action. Then we can rewrite the partition function as

$$Z = \int dE_p \exp[-S_{\text{eff}}(E_p,m,N_f,\beta,\kappa)], \tag{2.9}$$

where

$$S_{\text{eff}}(E_p,m,N_f,\beta,\kappa) = -\ln M(E_p,\kappa) - 6V\beta E_p + S_{\text{eff}}^F(E_p,m,N_f,\kappa) \tag{2.10}$$

is the full effective action.

The main effort to be paid is to calculate $S_{\text{eff}}^F(E_p,m,N_f,\kappa)$ through (2.7), where $\langle [\det\Delta(U)]^{N_f^{\text{latt}}} \rangle_{E_p}$ is the fermionic determinant averaged over the configurations with the probability distribution

$$\frac{\delta[S_p(U) - E_p] \exp[8V\kappa S_l(U,\phi)]}{M(E_p,\kappa)}. \tag{2.11}$$

These configurations are generated as follows.

(a) Starting from a gauge-scalar configuration $\{U,\phi\}$ with an energy E_p, generate microcanonically a gauge configuration $\{U'\}$:

$$U' = R_0^\dagger U^\dagger R_0^\dagger, \tag{2.12}$$

where $R_0 = R/|R|$ is an element of the gauge group, and R is the sum of six staples which surround the link U. The usage of the microcanonical process is to generate configurations with the probability distribution $\delta[S_p(U) - E_p]$, but it also decorrelates well the configurations. This trial configuration U' is accepted if

$$\exp[8V\kappa S_l(U',\phi) - 8V\kappa S_l(U,\phi)] > r, \tag{2.13}$$

where r is a random number. This is the feedback of the scalars to the gauge configurations.

(b) Change the scalar configuration $\{\phi'\}$ randomly. If

$$\exp[8V\kappa S_l(U',\phi') - 8V\kappa S_l(U',\phi)] > r', \tag{2.14}$$

where r' is another random number, then $\{\phi'\}$ is ac-

cepted. In order to decorrelate the scalar configurations, before going back to (a) for another new configuration, we perform several deterministic steps; i.e., for a given site x, make the update

$$\phi_x'' = -\phi_x + 2\frac{(B_x^\dagger \phi_x)}{|B_x^\dagger B_x|} B_x, \tag{2.15}$$

and let x go over all the lattice sites. Such a process does not change the link energy $S_l = \sum_x \mathrm{Re}(\phi_x^\dagger B_x)/(4V)$, where $B_x = \sum_\mu U_{x,\mu}\phi_{x+\mu}$.

There are several major advantages in this algorithm: (a) The effective fermionic action S_{eff}^F does not depend on β and its dependence on N_f can be easily obtained, which means for arbitrary β or N_f in an energy interval where the microcanonical quantities are known, it is not necessary to repeat the expensive part of the computation, i.e., the determination of $\lambda_i(U)$; (b) as seen in (2.8), S_{eff}^F as a function m (possibly including $m = 0$) can be obtained without repeating the microcanonical simulation; (c) the function integral over fermion, gauge, and scalar fields becomes a one-dimensional integral over the pure gauge energy E_p.

In one word, one can get the full effective action by only one microcanonical pure gauge simulation. From the previous investigations [5–9], we know that such a full effective action would give us a lot of information on the thermodynamical properties of the system and would be very useful for the phase structure analysis. The dynamics of the system can be investigated either by canonical simulations of the equivalent effective gauge-scalar model or by saddle-point technique as to be discussed in the following section.

III. SADDLE-POINT ANALYSIS

Since all three terms in the effective action (2.10) diverge linearly with V in the $V \to \infty$, the thermodynamics of the system in this limit can be analyzed using the saddle-point technique. The advantage is that once we know S_{eff}^F and $M(E_p,\kappa)$, we can obtain all the thermodynamical quantities for arbitrary (m, N_f, β) without further simulations.

The mean plaquette energy $\langle E_p\rangle = E_0(m, N_f, \beta, \kappa)$ is the saddle point, i.e., the solution to the saddle-point equation

$$\frac{-1}{\bar{M}(E_p,\kappa)}\frac{\partial \bar{M}(E_p,\kappa)}{\partial E_p} + \frac{\partial \bar{S}_{\mathrm{eff}}^F(E_p,m,N_f,\kappa)}{\partial E_p} - 6\beta = 0 \tag{3.1}$$

satisfying the minimum condition

$$\left\{\frac{1}{\bar{M}(E_p,\kappa)^2}\left[\frac{\partial \bar{M}(E_p,\kappa)}{\partial E_p}\right]^2 - \frac{1}{\bar{M}(E_p,\kappa)}\frac{\partial^2 \bar{M}(E_p,\kappa)}{\partial E_p^2} + \frac{\partial^2 \bar{S}_{\mathrm{eff}}^F(E_p,m,N_f,\kappa)}{\partial E_p^2}\right\}_{E_0(m,N_f,\beta,\kappa)} > 0, \tag{3.2}$$

where

$$\bar{M}(E_p,\kappa) = M(E_p,\kappa)^{1/V},$$

$$\bar{S}_{\mathrm{eff}}^F(E_p,m,N_f,\kappa) = \frac{S_{\mathrm{eff}}^F(E_p,m,N_f,\kappa)}{V} \tag{3.3}$$

are the normalized quantities. $\bar{M}(E_p,\kappa)$ can be directly evaluated by numerically integrating (3.1) from the data of the quenched gauge-scalar models:

$$-\ln \bar{M}(E_p,\kappa) = 6\int_0^{E_p} dE\beta(E, N_f = 0) + \mathrm{const.} \tag{3.4}$$

Here one sees again the advantage of the definition of the density of states (2.6): we do not have to do extra quenched simulations of the pure gauge model nor extra calculation of the "effective scalar action."

By looking for the minimum of the full effective action as a function of energy E_p at given m, N_f, β, and κ, we obtain $\langle E_p(m, N_f, \beta, \kappa)\rangle$. Other thermodynamical quantities can be obtained from the information of effective action at the saddle point. For example, the chiral condensate and link energy are given by

$$\langle \bar{\psi}\psi\rangle = -\frac{1}{V}\frac{\partial \ln Z}{\partial m} = -\left.\frac{\partial \bar{S}_{\mathrm{eff}}^F}{\partial m}\right|_{E_0(m,N_f,\beta,\kappa)}, \tag{3.5}$$

$$E_l = \left.\frac{1}{8V}\frac{\partial S_{\mathrm{eff}}}{\partial \kappa}\right|_{E_0(m,N_f,\beta,\kappa)} = \left.\frac{-1}{8\bar{M}(E_p,\kappa)}\frac{\partial \bar{M}(E_p,\kappa)}{\partial \kappa}\right|_{E_0(m,N_f,\beta,\kappa)} + \left.\frac{\partial \bar{S}_{\mathrm{eff}}^F(E_p,m,N_f,\kappa)}{8\partial \kappa}\right|_{E_0(m,N_f,\beta,\kappa)}. \tag{3.6}$$

The phase structure of the system is completely described by the behavior of the effective action as a function of the energy and of other parameters. For instance, nonanalytic behavior of the normalized density of states $\bar{M}(E_p,\kappa)$ (as in the quenched Higgs model) or the fermionic effective action $S_{\mathrm{eff}}^F(E_p,m,N_f,\kappa)$ could generate phase transitions.

IV. SIMULATIONS AND RESULTS

The most CPU time consuming part of the simulation is to compute the effective fermionic action S_{eff}^F defined by (2.7). In practice, the algorithm is implemented in the following way.

(a) Choose some fixed κ.

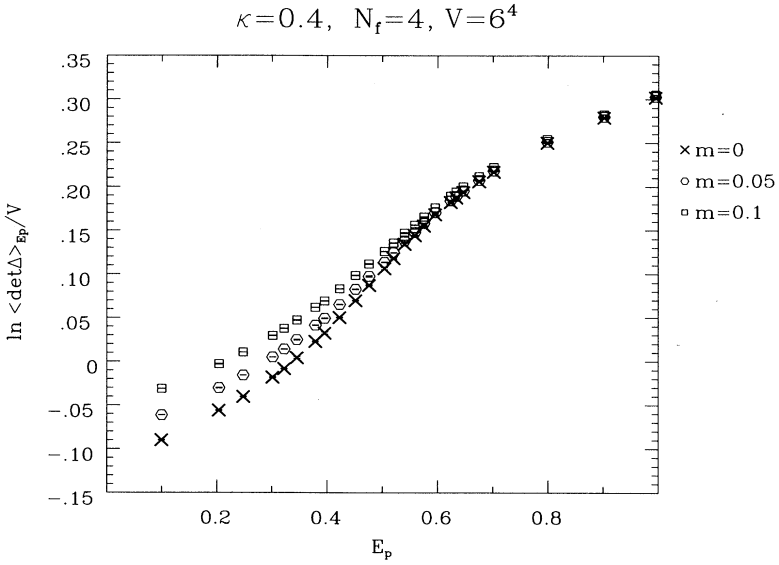

FIG. 1. $-\bar{S}^F_{\rm eff}$ as a function of E_p.

(b) Generate configurations $\{U,\phi\}$ at the desired energy E_p as described above, where the configurations can be decorrelated by many microcanonical updates.

(c) Once a decorrelated configuration $\{U,\phi\}$ is generated, calculate all the positive eigenvalues $\lambda_i(U)$ of the massless fermionic matrix by the Lanczos algorithm.

(d) Averaging the fermionic determinant over the decorrelated configurations, we get the effective fermionic action for the given E_p and arbitrary bare parameter m and N_f. Repeating (b)–(d) for different E_p, we get $S^F_{\rm eff}$ at the chosen κ, and arbitrary m and N_f as a function of E_p by interpolation.

Other detailed techniques, like the microcanonical update for the gauge field, diagonalization of the fermionic matrix, and systematic analysis of the effective fermionic action, can be found in [2–4].

To see how well the algorithm works, let me concentrate on a prototype of the fermion-gauge-scalar models with U(1) gauge group, a scalar of fixed modulus, and one staggered fermion ($N_f^{\rm latt} = N_f/4 = 1$), where both the scalar and fermion have charge one [1,10].

We have done detailed simulations using the algorithm described in Sec. II on 6^4, 8^4, and $6^3 16$ lattices for $\kappa = 0.4, 0.6, 0.8, 1.15$, where the 6^4 lattice has the best statistics. On each lattice, ~ 300 decorrelated configurations $\{U,\phi\}$ are generated in the pure gauge energy range $E_p \in [0,1)$ and their massless fermionic matrix is diagonalized, from which we construct the effective fermionic action $S^F_{\rm eff}$ as a function of the bare parameters m, N_f. (For some interesting points, 600 decorrelated configurations are generated.)

Here we would discuss only the results at $\kappa = 0.4$ on the 6^4 lattice. Figure 1 shows $-\bar{S}^F_{\rm eff} = \ln\langle\det\Delta\rangle_{E_p}/V$ as a function of E_p for several fermion masses. From the quenched simulation, we obtain the first term in (2.10), that is $-\ln\bar{M}(E_p,\kappa)$, as plotted in Fig. 2. Then we use the saddle-point technique described in Sec. III to calcu-

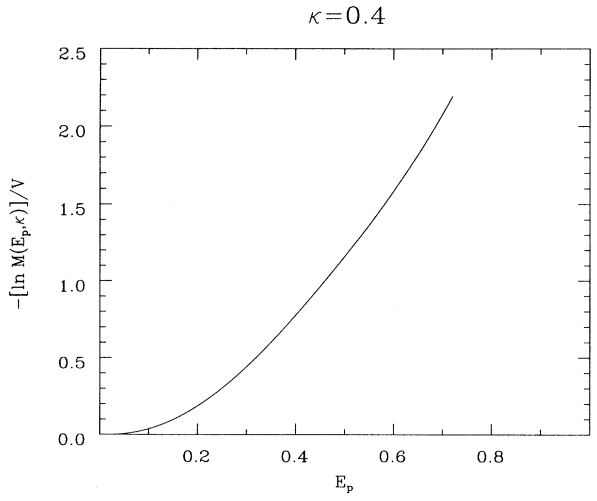

FIG. 2. $-\ln\bar{M}(E_p,\kappa)$ as a function of E_p.

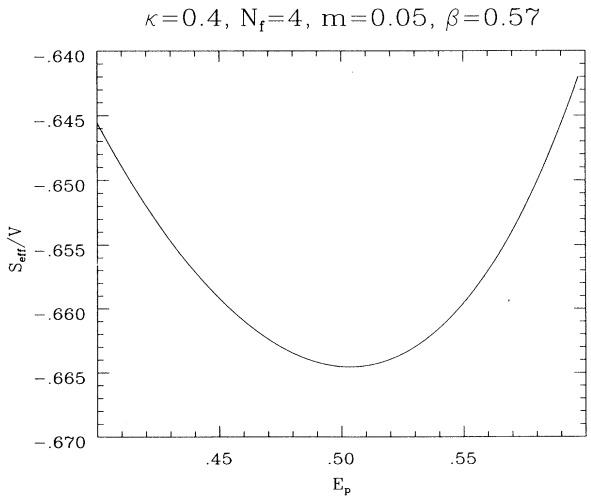

FIG. 3. The normalized full effective action as a function of E_p.

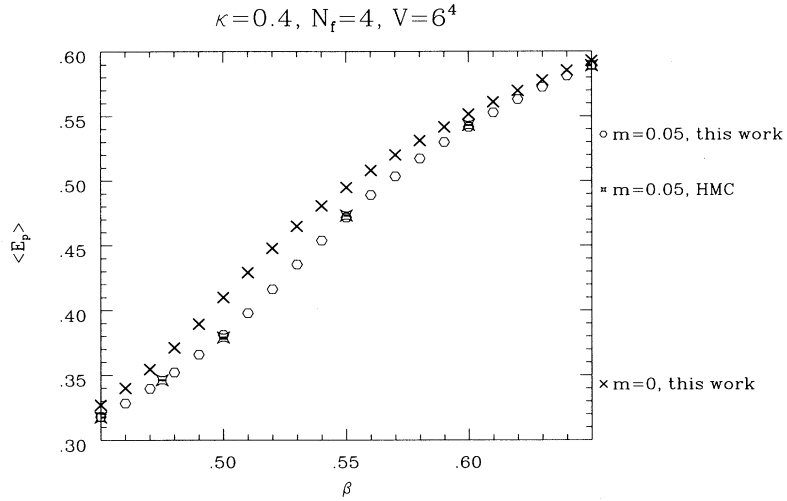

FIG. 4. Mean plaquette energy as a function of β.

late the expectation value for the plaquette energy $\langle E_p \rangle$ by locating the minimum of the full effective action as a function of E_p: $E_0(m, N_f, \beta, \kappa)$. An example is plotted in Fig. 3. According to the saddle-point arguments, the mean plaquette energy $\langle E_p \rangle$ is just $E_0(m, N_f, \beta, \kappa)$, with dependence on β shown in Fig. 4. Other thermodynamical quantities like the link energy and chiral condensate as a function of β, shown in Figs. 5 and 6, are the corresponding microcanonical quantities at $E_p = E_0(m, N_f, \beta, \kappa)$. For finite m, we also compare $\langle E_p \rangle$, $\langle E_l \rangle$, and $\langle \bar{\psi}\psi \rangle$ with those from the HMC simulations and find that they are in perfect agreement, which means our algorithm is supported by the exact algorithm. The HMC data for various m and κ are satisfactorily reproduced as well.

Now let me discuss the chiral limit, which could also be accessible by this algorithm. The results for $\langle E_p \rangle$ and $\langle E_l \rangle$ at $m = 0$ are also shown in Figs. 4 and 5. Of course, the accessibility to the chiral limit should be further checked by comparing results for more quantities from different algorithms. Whereas $\langle \bar{\psi}\psi \rangle$ vanishes identically and mass extrapolation has to be done, the chiral susceptibility [10,11] at $m = 0$ is calculable and serves as a more useful order parameter for the chiral transition. Again, the critical points are consistent with those obtained from HMC on the same lattice. Detailed analysis of the chiral susceptibility and comparison with the HMC data have been reported elsewhere [10].

V. DISCUSSIONS

The algorithm [2–4] and some techniques have been generalized to the fermion-gauge-scalar models, which allow us to search the parameter space (m, N_f, β) with much lower computer cost than the conventional algorithms; therefore, it is very suitable for the phase structure analysis. The essential ingredients are the new and appropriate definitions of the density of states and the effective fermionic action when the scalar field is included. Our algorithm and HMC give consistent results at finite bare mass $m \neq 0$. Some results from this algorithm in the chiral limit $m = 0$ have also been presented. An interesting application of this algorithm is to determine chiral

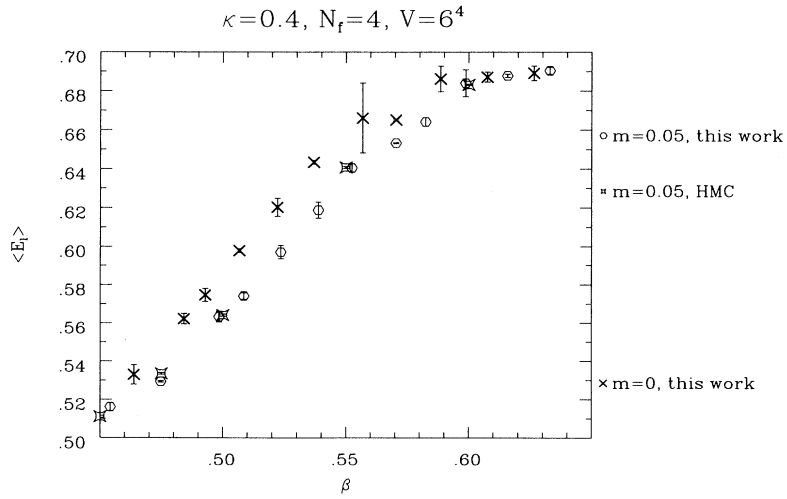

FIG. 5. Link energy as a function of β.

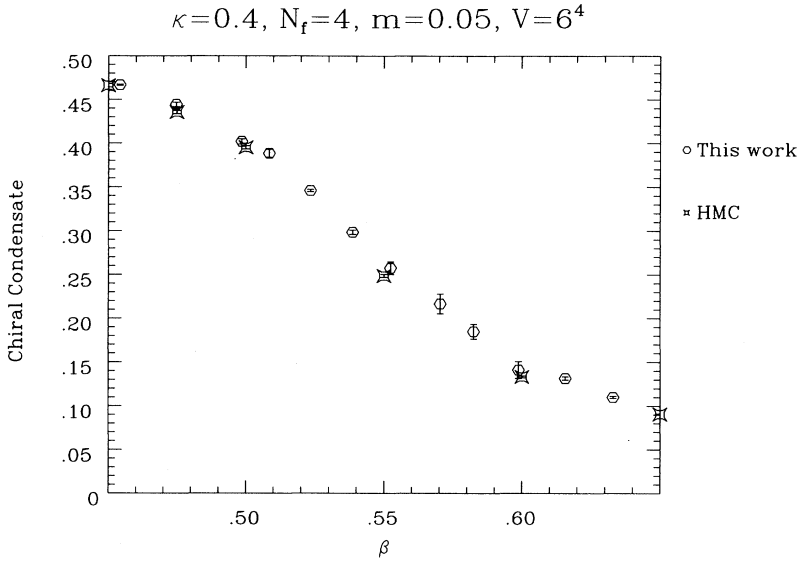

FIG. 6. Chiral condensate as a function of β.

transition line in a strongly coupled fermion-gauge-scalar model [10,11].

While having demonstrated the advantages of the algorithm on the 6^4 lattice, we would like to mention some open questions. For large lattice volumes, it is time and memory consuming to diagonalize the fermionic matrix. For example, on the 8^4 lattice, the amount of data required grow so fast that the results have not been well tested. Although the Lanczos algorithm is parallelizable [4] and may be vectorizable, we had not vectorized it when the algorithm was implemented. It is not easy to evaluate observables other than the thermodynamical quantities. These problems are under further investigation.

Concerning the possible extension to the Yukawa models, here we would like to give some brief discussions. These models are described by

$$S = -8V\kappa S_l(\phi) + S_f(\phi,\psi) \tag{5.1}$$

with

$$S_l(\phi) = \frac{1}{4V}\sum_{x,\mu}\mathrm{Re}(\phi_x^\dagger\phi_{x+\mu}),$$

$$S_f(\phi,\psi) = \bar{\psi}\Delta(\phi)\psi, \tag{5.2}$$

where instead of gauge-fermion interactions in (2.2), we have fermion-scalar interactions

$$\Delta(\phi) = \not{\partial}^{\mathrm{latt}} + y(\phi_x P_R + \phi_x^\dagger P_L) \tag{5.3}$$

with y being the Yukawa coupling, and P_R and P_L being the right-hand and left-hand projectors, respectively. The absence of the gauge field $U = 1$ in S_l makes it possible to microcanonically update the configurations by (2.15) without changing S_l. Again, such a process is expected to reduce the fluctuations in $\det\Delta(\phi)$. Now the partition function is

$$Z = \int dE_l M(E_l)\exp(8V\kappa E_l)\exp[-S_{\mathrm{eff}}^F(E_l,m,N_f,y)], \tag{5.4}$$

where

$$M(E_l) = \int [d\phi][d\phi^\dagger]\delta(S_l - E_l) \tag{5.5}$$

and

$$\exp[-S_{\mathrm{eff}}^F(E_l,m,N_f,y)] = \frac{\int[d\phi][d\phi^\dagger]\delta(S_l-E_l)[\det\Delta(\phi)]^{N_f^{\mathrm{latt}}}}{M(E_l)}. \tag{5.6}$$

The diagonalization of the fermionic matrix can be done in a way similar to that in [12]. An advantage now is that the parameter space (m, N_f, κ) can be economically searched.

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