BOSONIZED DYNAMICAL FERMIONS IN 3+1 DIMENSIONS

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A numerical method based on the Jordan–Wigner representation of anticommuting variables is developed in 3+1 dimensions for Wilson fermions. Detailed tests are performed in the case of free fermions. The application to interacting quantum field theories is discussed.

Anticommuting Grassmann variables can be dealt with numerically in the Jordan–Wigner representation [1]. Although this fact is well known for a long time, relatively little is known about the possibility of using this representation in Monte Carlo simulations of fermionic quantum field theories. The extension of its applications in (1+1)-dimensional systems [2] to interesting higher-dimensional models seems difficult, due to the appearance of the appearance of sign factors and complex matrix elements [3]. Recently Duncan suggested a new method for the numerical simulation of higher-dimensional fermionic quantum fields based on the Jordan–Wigner representation [4]. The method was tested for free staggered fermions [5] in 2+1 dimensions. In the present letter some modifications are suggested which are relevant for applications in (3+1)-dimensional interacting systems. Detailed tests are performed with free Wilson fermions [6] and the inclusion of interactions with bosonic fields is discussed on the example of a simple scalar–fermion theory with Yukawa coupling.

The Grassmann algebra ($m, n = 1, 2, ..., N$)

$$\{c_m^\dagger, c_n\} = \delta_{m,n}, \quad \{c_m, c_n\} = \{c_m^\dagger, c_n^\dagger\} = 0 \tag{1}$$

is realized in the Jordan–Wigner representation by

$$c_n = \sigma_3^{(1)} \sigma_3^{(2)} ... \sigma_3^{(n-1)} \sigma_-^{(n)} ,$$
$$c_n^\dagger = \sigma_3^{(1)} \sigma_3^{(2)} ... \sigma_3^{(n-1)} \sigma_+^{(n)} . \tag{2}$$

Here $\sigma_j^{(n)}$, $n = 1, ..., N$, $j = 1, 2, 3$ denote Pauli matrices which commute for different n:

$$[\sigma_j^{(m)}, \sigma_k^{(n)}] = 2i\delta_{m,n} \epsilon_{jkl} \sigma_l^{(m)} \tag{3}$$

and, as usual

$$\sigma_\pm = \tfrac{1}{2}(\sigma_1 \pm i\sigma_2) . \tag{4}$$

It can be shown that every representation of the Grassmann algebra in a separable Hilbert space is unitarily equivalent to this. For a quadratic Hamilton operator one needs the relation

$$c_m^\dagger c_n = \sigma_+^{(m)} \sigma_-^{(n)} \rho(m, n) , \tag{5}$$

where $\rho(m, n) = \rho(n, m)$ is given by

$$\rho(m, m) = 1, \quad \rho(m, m+1) = -1 ,$$
$$\rho(m, m+k) = -\sigma_3^{(m+1)} \sigma_3^{(m+2)} ... \sigma_3^{(m+k-1)} . \tag{6}$$

For a Dirac fermion field the anticommuting variables can be denoted by $\psi_{\alpha x}$, where $\alpha = 1, 2, 3, 4$ is the Dirac index and x the lattice point in 3-dimensional space. The Hamilton operator for free Wilson fermions with mass m is

$$H = \sum_x \psi_x^\dagger m \beta \psi_x - \frac{r}{2} \sum_{x,k} (\psi_{x+\hat{k}}^\dagger \beta \psi_x + \psi_x^\dagger \beta \psi_{x+\hat{k}})$$
$$+ \frac{i}{2} \sum_{x,k} (\psi_{x+\hat{k}}^\dagger \alpha_k \psi_x - \psi_x^\dagger \alpha_k \psi_{x+\hat{k}}) . \tag{7}$$

The summation $\sum_k$ goes over the three orthogonal directions. $\hat{k}$ is the unit vector in direction k and in a $2 \otimes 2$ block notation the Dirac matrices β, α_k are

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} . \tag{8}$$

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In the continuum limit the second term in the hamiltonian, which is proportional to the Wilson parameter $0<r\leqslant 1$, removes the additional lattice fermion species form the spectrum. $r=0$ corresponds to "naive" lattice fermions. Using eq. (5) one obtains the hamiltonian in the Jordan–Wigner representation. Let us consider here, for simplicity, only the case of naive fermions. In this case we have

$$H=\sum_{\alpha,x} m\lambda_\alpha \sigma_+^{(\alpha x)}\sigma_-^{(\alpha x)} + \frac{1}{2}\sum_{\alpha,x,k}[\lambda(\alpha,k)\sigma_+^{(\gamma(\alpha,k)x+\hat{k})}\sigma_-^{(\alpha x)} \times\rho(\gamma(\alpha,k)x+\hat{k},\alpha x)+\text{h.c.}], \tag{9}$$

where $\lambda_1=\lambda_2=-\lambda_3=-\lambda_4=1$ and $\lambda(\alpha,k)$ and $\gamma(\alpha,k)$ are given in a matrix form by

$$\lambda(\alpha,k)=\begin{pmatrix} i & -1 & +i\\ i & +1 & -i\\ i & -1 & +i\\ i & +1 & -i\end{pmatrix},$$

$$\gamma(\alpha,k)=\begin{pmatrix} 4 & 4 & 3\\ 3 & 3 & 4\\ 2 & 2 & 1\\ 1 & 1 & 2\end{pmatrix}. \tag{10}$$

The fermion variables are represented in the computer by a single bit. The order of these variables has some relevance due to the sign factor ρ appearing in eq. (5). In the case of Wilson fermions it is reasonable to store the four Dirac components belonging to a lattice site consecutively. The sites can be stored in the usual lexicographic order. The very specific order used in ref. [4] is not necessary. Arbitrary boundary conditions are possible. In the present paper always periodic boundary conditions are assumed. Of course, on the boundaries the phase factor $\rho(...x+\hat{k},...x)$ is sometimes given by a longer product than inside the lattice. These phase factors have to be often computed during the simulation, therefore it is advantageous to keep them short. In the way just described the average work per site needed to compute them everywhere on an L^3 lattice is growing with L^2.

The aim of the simulation is to compute traces like

$$Z=\mathrm{Tr}\exp(-\beta H), \tag{11}$$

with $\beta\equiv T^{-1}$ the inverse temperature. Following ref. [4] this is done on $L^3\cdot L_0$ asymmetric lattices, where $\beta=a_0L_0$. The lattice is much finer in the "time" direction, therefore the ratio of the lattice spacings a_0 is much smaller than 1. Up to first order in a_0 one can replace

$$\mathrm{Tr}\exp(-L_0a_0H) \rightarrow \mathrm{Tr}\{\exp(-a_0H_\mathrm{D})\,(1-a_0H_\mathrm{R})\}^{L_0}. \tag{12}$$

Here $H=H_\mathrm{D}+H_\mathrm{R}$ is a decomposition of the hamiltonian into a diagonal piece H_D and the rest H_R containing the off-diagonal terms in the fermionic variables. In ref. [4] $H_\mathrm{D}=0$ and $H_\mathrm{R}=H$ was taken, but the more general form in (12) allows the combination of the fermionic algorithm with the usual Monte Carlo integration procedure for the bosonic variables. Namely, in the case of interacting theories the bosonic piece of the hamiltonian can be added to H_D (see later). Also in the case of purely fermionic theories, as a numerical comparison shows, the partly exponential form in eq. (12) turns out better from the point of view of the autocorrelation of subsequent configurations. Another advantage of eq. (12) is that it is insensitive to a constant shift in the hamiltonian, because the constant is contributing to H_D and therefore drops out from the relative probability defining the heat bath procedure (see below). This is not so for $H_\mathrm{D}=0$ when a careful choice of the constant is usually necessary, even if at the end (for $a_0\rightarrow 0$) the dependence on it has to disappear.

In the specific case of free Wilson fermions the diagonal part is given by

$$H_\mathrm{D}|\{\xi\}\rangle = mA\{\xi\}|\{\xi\}\rangle, \tag{13}$$

where $\{\xi\}=\{\xi(\alpha,x),\ \alpha=1,2,3,4,\ x=1,...,L^3\}$ with $\xi(\alpha,x)=\pm 1$ denotes the fermion variables, $|\{\xi\}\rangle$ is the state in the Hilbert space belonging to $\{\xi\}$ and

$$A\{\xi\}\equiv\sum_{\alpha,x}\lambda_\alpha\delta_{1,\xi(\alpha,x)}. \tag{14}$$

In this notation, after inserting in eq. (12) the complete set of states L_0 times, we have

$$Z=\sum_{\{\xi\}_1,...\{\xi\}_{L_0}}\prod_{t=1}^{L_0}\{\exp[-a_0mA\{\xi\}_t] \times\langle\{\xi\}_t|1-a_0H_\mathrm{R}|\{\xi\}_{t+1}\rangle\}^{L_0}+..., \tag{15}$$

where the dots are small corrections due to the replacement in (12) and, by definition, $\{\xi\}_{L_0+1}\equiv\{\xi\}_1$.

The non-zero contributions in the sum (15) correspond to sequences $\{\xi\}_1 ... \{\xi\}_{L_0}$ such that the consecutive states $\{\xi\}_t$ and $\{\xi\}_{t+1}$ differ at most by a flip of a single "active fermion link". A "fermion link" is a pair of fermion variables connected by a non-zero off-diagonal matrix element of H_R. A fermion link is active if the fermion variable pair is unequal. The sum in eq. (15) is performed by sampling with a heat bath Monte Carlo. The probability of a configuration is taken to be proportional to

$$P(\{\xi\}_1 ... \{\xi\}_{L_0}) = \prod_{t=1}^{L_0} \exp(-a_0 m \Lambda \{\xi\}_t) \times |\langle \{\xi\}_t | 1 - a_0 H_R | \{\xi\}_{t+1} \rangle| . \quad (16)$$

A heat bath step consists of keeping the states $|\{\xi\}_{t-1}\rangle$ and $|\{\xi\}_{t+1}\rangle$ fixed and choosing $|\{\xi\}_t\rangle$ with relative probability

$$W(\{\xi\}_t) = \exp(-a_0 m \Lambda \{\xi\}_t) \times |\langle \{\xi\}_{t-1} | 1 - a_0 H_R | \{\xi\}_t \rangle \times \langle \{\xi\}_t | 1 - a_0 H_R | \{\xi\}_{t+1} \rangle| . \quad (17)$$

Since the probability P is defined in eq. (16) by the absolute value of matrix elements, the partition function in (15) is given by

$$Z = \left\langle \prod_{t=1}^{L_0} \frac{\langle \{\xi\}_t | 1 - a_0 H_R | \{\xi\}_{t+1} \rangle}{|\langle \{\xi\}_t | 1 - a_0 H_R | \{\xi\}_{t+1} \rangle|} \right\rangle_P . \quad (18)$$

Here $\langle \ \rangle_P$ means an expectation value in the Monte Carlo process defined by the probability P. The expectation value of some operator can also be obtained similarly. As a simple example one can calculate the expectation value of $\bar{\psi}_x \psi_x$ by inserting this operator, for instance, at the first timeslice $t = 1$:

$$\langle \bar{\psi}_x \psi_x \rangle = Z^{-1} \left\langle \sum_\alpha \lambda_\alpha \delta_{1,\xi(\alpha x)_1} \times \prod_{t=1}^{L_0} \frac{\langle \{\xi\}_t | 1 - a_0 H_R | \{\xi\}_{t+1} \rangle}{|\langle \{\xi\}_t | 1 - a_0 H_R | \{\xi\}_{t+1} \rangle|} \right\rangle_P . \quad (19)$$

The Monte Carlo step determined by the relative probability W in (17) does not change the exactly conserved quantum numbers like, for instance, the fermion number. In order to sum over all the sectors belonging to different quantum numbers one has to choose the intial configuration randomly and repeat the Monte Carlo summation many times. Of course, it is also possible to stay, for instance, at some given fermion number if one is interested only in such averages.

As a first test of the method I performed Monte Carlo simulations of a free Wilson- (or naive-) fermion field with the hamiltonian in eq. (9). The aim was to compare the results on $\langle \bar{\psi}\psi \rangle$ to the exact value at given inverse temperature β, namely

$$\langle \bar{\psi}_x \psi_x \rangle = -\frac{2}{L^3} \sum_q \frac{\sinh(\beta E_q)\ (m - r \sum_l \cos q_l)}{E_q [1 + \cosh(\beta E_q)]} . \quad (20)$$

Here $\sum_q$ means a momentum sum over the Brillouin zone corresponding to periodic boundary conditions and E_q is the energy belonging to momentum q:

$$E_q \equiv \sqrt{\left(m - r \sum_l \cos q_l\right)^2 + \sum_l \sin^2 q_l} . \quad (21)$$

The first question is, of course, the dependence of the numerical results on the timelike asymmetry of the lattice a_0. The replacement in eq. (12) implies that the exact trace is obtained only in the limit $a_0 \to 0$. The computed values of $\langle \bar{\psi}\psi \rangle$ on a 4^4 lattice (which means actually $L^3 \cdot \beta$ with $L = \beta = 4$ and therefore $L_0 = \beta / a_0$ timeslices) for free naive fermions ($r = 0$) are shown in fig. 1. As can be seen, the deviation from the exact value at $a_0 = 0$ is nearly linear in a_0 for small a_0. The deviation becomes smaller than the statistical error for $a_0 = \frac{1}{320}$ (i.e. $L_0 = 1280$). The statistics corresponds typically to 5000 sweeps per a_0 value after 1000 equilibrating sweeps (a "sweep" means on the average one heatbath change per fermionic variable on the $L^3 \cdot L_0$ lattice). The statistical errors were always estimated by the usual binning of the sequence of results (in our case into bins of length 2^n).

The order of magnitude of the deviation from the exact value of the trace can be understood by comparing $\exp(-L_0 a_0 E)$ to $(1 - a_0 E)^{L_0}$. Assuming $E \simeq 1$ for the magnitude of the energy eigenvalue, the deviation of the two expressions can easily be seen to be of the order of $(a_0 L_0)^2 / L_0 = a_0 \beta$. This is linear in a_0 and is of the same order of magnitude as the deviations in fig. 1. It is obvious from here that a substantial improvement can be expected from the second order replacement $\exp(-L_0 a_0 E) \to (1 - a_0 E + \frac{1}{2} a_0^2 E^2)^{L_0}$. In order to achieve the same approximation it is enough to have typically by a factor of more

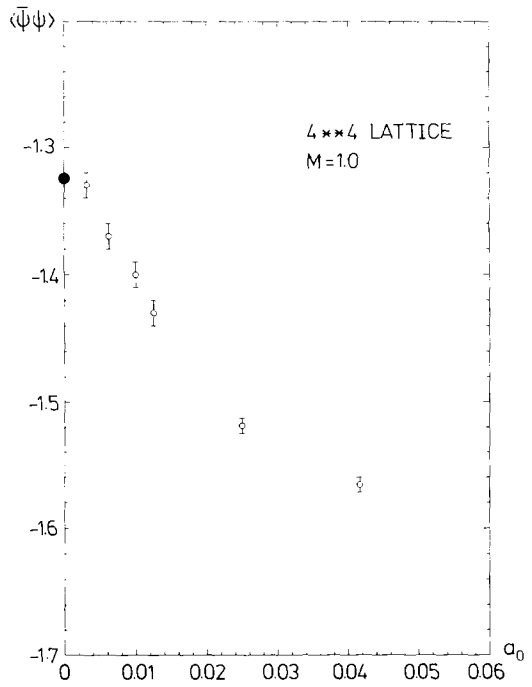

Fig. 1. The dependence of $\langle\bar{\psi}\psi\rangle$ on the ratio of the timelike to spacelike lattice spacing a_0 for free naive fermions with mass in lattice units $m=1.0$. The spacelike lattice is 4^3 and the inverse temperature $\beta=4$. [This can be shortly referred to as a 4^4 lattice, although the calculation is actually done on a $4^3\cdot(4/a_0)$ lattice.] The dot at $a_0=0$ is the exact result from eq. (20).

than 10 smaller L_0. The second order analogue for the replacement in eq. (12) is

$$\mathrm{Tr}\exp(-L_0 a_0 H) \rightarrow \mathrm{Tr}\{\exp(-a_0 H_D)\ (1-a_0 H_R+\tfrac{1}{2}a_0^2 H_R^2)\}^{L_0}. \tag{22}$$

The computer code for this quadratic formula can be substantially more complicated than for the linear one, but the expected reduction of the time length of the lattice will probably lead to considerable gain in performance. (In the present calculations always the linear approximation was used.)

The initial configurations were randomly chosen out of all possible time-independent configurations. It can be shown that in $a_0\to 0$ limit this is a correct procedure, although there also non-zero configurations which cannot be reached from this by subsequent heat bath steps. As was stated before, a non-zero contribution is obtained from a sequence $\{\xi\}_1\ldots\{\xi\}_{L_0}$ if the subsequent states are either identical or differ at most by a flip of a single active fermion link. Due to the periodicity the configuration has to be the same after going around once in time direction. Therefore, either the subsequent flips have to compensate each other or otherwise the same state can also be achieved if a change is "going around the world" in space. These later sequences have, however, a minimum number of L factors of a_0 in the probability and hence are negligible for $a_0\to 0$.

A potential source of problems in the calculation of expectation values is that the phase factors in the nominator and denominater [as in eqs. (18), (19)] can strongly oscillate and make the convergence to the average slow. No such problems exist for the free Wilson fermions and for the scalar–fermion model discussed below. Moreover, the expectation value in eq. (18) determining Z is in these cases exactly 1. As a manner of fact, I saw this property first in the numerical calculation and then could verify it for large

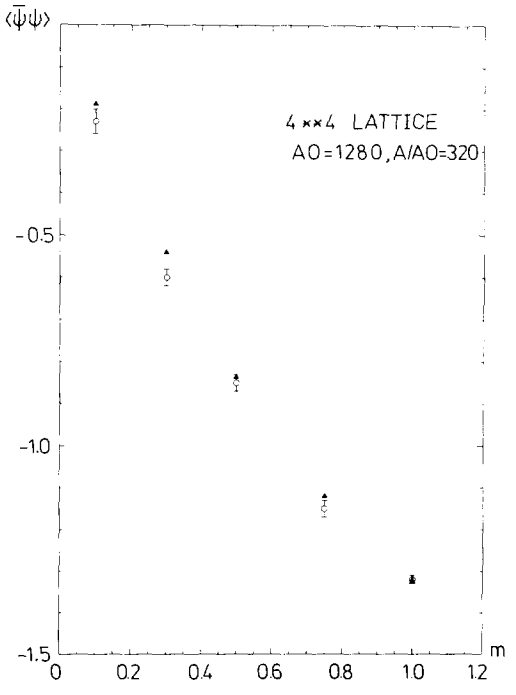

Fig. 2. $\langle\bar{\psi}\psi\rangle$ as a function of the mass m in lattice units on 4^4 lattice for free naive fermions with $a_0=\frac{1}{320}$. The Monte Carlo results are compared to the exact values from eq. (20) shown by the triangles.

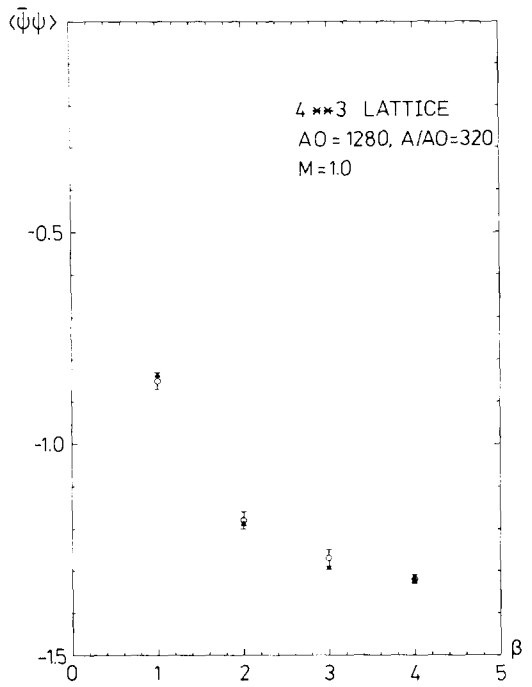

Fig. 3. The same as fig. 2 as a function of the inverse temperature β.

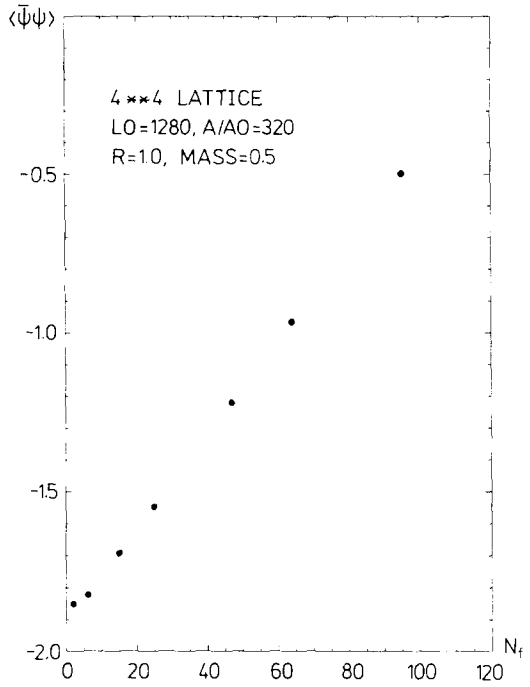

Fig. 4. The same as fig. 2 as a function of the fermion number N_f for Wilson fermions with $r=1$ and $m=3.5$. The mass in the fermion propagator is $m-3r=0.5$.

classes of configurations in the specific representation of Dirac matrices (8) and for the chosen ordering of fermion variables. Note that this is apparently different for free staggered fermions in 2+1 dimensions with free boundary conditions, because according to ref. [4] there we have $Z\neq 1$.

The dependence of $\langle\bar{\psi}\psi\rangle$ on the fermion mass (m), on the inverse temperature (β) and on the fermion number (N_f) is shown in figs. 2–4. The spacelike lattice is always 4^3 and the asymmetry parameter $a_0=\frac{1}{320}$. Fig. 4 is for Wilson fermions with $r=1$, otherwise naive fermions corresponding to $r=0$ were taken. The statistics in figs. 1–3 is typically 5000 sweeps after 1000 equilibrating sweeps. Fig. 4 has by a factor of 4 more statistics. As one can see in figs. 2 and 3, the exact values given by eq. (20) are well reproduced. Fig. 4 could be compared to the value obtained by approximating the fixed fermion number by fixed chemical potential as is usually done in macroscopic systems. On the small lattice this would, however, involve a non-negligible error.

Let us note that the exact result in eq. (20) refers to the sum over fermion number. As discussed before, this can be obtained in principle by performing a sequence of simulations with randomly chosen initial configurations and averaging over the results. However, in the sum in eq. (20) the states with small fermion number dominate (the chemical potential is zero). In addition, for naive fermions $\langle\bar{\psi}\psi\rangle$ is slowly varying near zero fermion number (actually, slower than for Wilson fermions with $r=1$ on fig. 4), therefore a single simulation with small fermion number gives already a good estimate. This is how figs. 1–3 were obtained, in order to save computer time.

By the use of eqs. (12) and (22) the extension of the updating procedure to scalar–fermion theories with Yukawa couplings becomes possible. As a simple example I considered a single-component scalar field ϕ_x coupled to a Wilson-fermion field by the Yukawa coupling $G\phi_x\bar{\psi}_x\psi_x$. Since in the representation (8) the Yukawa coupling is diagonal in the fermion variables, it can be added to H_D together with the purely scalar piece of the action. The updating of the fermion variables is the same as before (the only difference is the fluctuating mass term implied by the

varying scalar field). The updating of the scalar field can be done by the usual Monte Carlo procedure with H_D as the action. Since the lattice spacing is smaller in the time direction, the scalar hopping parameter has to be different in spacelike and timelike directions. The ratio of the two has to be tuned in such a way that euclidean rotation invariance be restored in the continuum limit. (For the similar problem with gauge fields on asymmetric lattices see e.g. ref. [7].) The convergence of the Monte Carlo procedure on small lattices (between 4^4 and 8^4) turned out to be similar to the free case. More details about the simulation of this scalar–fermion model will be published later [8].

It is important to note that the $a_0 \to 0$ extrapolation is generally not necessary. One can also work with small but finite a_0 which corresponds to an action $H_D - a_0^{-1} \log(1 - a_0 H_R)$. This contains some higher-order correction terms in addition to $H_D + H_R$, but in the euclidean invariant continuum limit these corrections probably do not matter.

The extension of this updating procedure to other scalar–fermion models and to models involving gauge fields seems possible but the efficiency of the method has to be seen in future investigations.

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