SIMULATION OF STAGGERED FERMIONS BY POLYMER AVERAGING

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A numerical fermion algorithm is developed in the framework of the polymer representation of the euclidean fermion path integral. It is based on a general Monte Carlo summation procedure which is applicable also in the case of oscillating phases. Tests are performed on four dimensional free staggered fermions.

The numerical simulation of four dimensional quantum field theories with fermions is difficult because of the Pauli exclusion principle. The standard way of taking into account the effect of the fermionic fields goes through the effective bosonic action containing the logarithm of the "fermion determinant" (for a recent review see ref. [1]). The disadvantage of this method is that it is relatively slow, due to the non-local character of the fermion determinant and, even worse, it is only applicable if the fermion determinant is positive. Examples where the fermion determinant is complex are, for instance: QCD with non-zero chemical potential or some simple scalar-fermion models with Yukawa couplings, etc. Alternative fermion methods can be formulated in the hamiltonian approach on the occupation number basis [2] or in the euclidean approach in the polymer representation [3]. These methods are, in principle, universally applicable. The problem is that they usually lead to a representation of the fermionic path integral as a sum of terms with different non-trivial phases and, therefore, are not directly suitable for an importance sampling Monte Carlo process. The straightforward possibility of taking into account the absolute value of different terms in the Monte Carlo process and including the phase in the measurable quantities is not practicable, because the phase factor in different regions can fluctuate independently and, therefore, its expectation value goes to zero exponentially with the volume. The numerical determination of these very small expectation values is practically not possible.

In the present paper I consider a more general Monte Carlo procedure which avoids the very small expectation values by averaging over equivalence classes of configurations. As a test case four-dimensional free Kogut–Susskind staggered fermions [4] will be considered in the euclidean polymer representation, where the phase factor is simply $+1$ or -1. Studies for Wilson fermions [5] and with non-vanishing interactions will be published later [6].

Let us first consider the general case with a set of bosonic fields represented by U and the discrete fermionic configurations denotes by z. (The notations are introduced here in the euclidean formulation, but the corresponding formulae in the hamiltonian approach with summation over occupation numbers can be obtained by a simple translation.) The partition function Z can be written as

$$Z = \int [dU] \sum_{z \in C} R(z, U) \exp[-S_b(U)] . \tag{1}$$

Here R is the contribution of the fermion configuration z, C stands for the set of all possible fermion configurations and S_b is the purely bosonic part of the euclidean action. The fermionic contribution R can be split into the absolute value $P(z, U)$ and the phase (or sign) $S(z, U)$:

$$R(z, U) = P(z, U)S(z, U) . \tag{2}$$

Performing a Monte Carlo integration (over U) and summation (over z) by the positive probability measure $P \exp(-S_b)$, the partition function is obtained as the expectation value of the phase factor:

$$Z = \langle S(z, U) \rangle_{P \exp(-S_b)} . \tag{3}$$

Let us note that there is nothing special in choosing the decomposition (2) just in this way. Other possibilities where the positive factor P is not equal to the absolute value of the fermionic contribution and the deviation is compensated by the factor S containing the phase may sometimes be better from the practical point of view (see later). The following formulae are valid in the general case. The expectation value of a generic quantity A is given by the ratio

$$\langle A \rangle = \frac{\langle A(z, U) S(z, U) \rangle_{P \exp(-S_b)}}{\langle S(z, U) \rangle_{P \exp(-S_b)}} . \tag{4}$$

As discussed before, this representation of the expectation values is, although mathematically correct, practically not useful. In order to obtain a better expression let us divide the set of fermion configurations in equivalence classes

$$C = \bigcup_\alpha C_\alpha \tag{5}$$

and consider the averages of the phase factor over the subsets C_α:

$$\bar{S}_{P\alpha}(U) \equiv \frac{\sum_{z \in C_\alpha} P(z, U) S(z, U)}{\sum_{z \in C_\alpha} P(z, U)} . \tag{6}$$

This can also be considered as a function of z defined on the whole configuration set C, if for every $z \in C_\alpha$ the average value in C_α is taken. This "averaged phase factor" will be denoted by $\bar{S}_{P\alpha}(z, U)$.

The averaged phase factor can also be split into its absolute value $\bar{P}$ and a phase:

$$\bar{S}_{P\alpha}(z, U) = \bar{P}_{P\alpha}(z, U) s(z, U) . \tag{7}$$

Similarly, the average of the product of a physical quantity with the phase factor can be written as

$$\overline{AS}_{P\alpha}(z, U) \equiv \frac{\sum_{z \in C_\alpha} P(z, U) A(z, U) S(z, U)}{\sum_{z \in C_\alpha} P(z, U)}$$

$$\equiv \bar{S}_{P\alpha}(z, U) a(z, U) . \tag{8}$$

In this case the expectation value (4) of the quantity A is given by

$$\langle A \rangle = \frac{\langle a(z, U) s(z, U) \rangle_{P \exp(-S_b) \bar{P}}}{\langle s(z, U) \rangle_{P \exp(-S_b) \bar{P}}} \tag{9}$$

where the Monte Carlo summation is performed by

the probability $P \exp(-S_b) \bar{P}$. Up to now this procedure is completely general. Its success in solving the problem of oscillating phases depends on finding a proper definition of equivalence classes of states. A good definition is such that the phase fluctuation of the average is strongly reduced, in an ideal case completely removed: $s(z, U) \equiv +1$. Another aspect for a good choice of equivalence classes is that the evaluation of $a(z, U)$ in eq. (8) should be simple. The best case is if the value of important physical quantities is the same in the whole equivalence class. In the example discussed below this is true, for instance, if the quantity is determined by the number of monomers. More generally, for the calculation of fermionic expectation values some additional open lines have to be introduced in the polymer configuration [3]. The contribution of a configuration is usually determined by the positions of the endpoints of these lines, therefore a simple equivalence relation should not change these endpoints. A more detailed discussion of the calculation of typical fermionic expectation values will be given in a future publication [6].

In order to test the applicability of this general method in four dimensional quantum field theories I first considered free staggered and Wilson fermions both in the euclidean invariant polymer representation [3] and in the linear approximation to the hamiltonian method on the occupation number basis [7,8]. The problem of oscillating phases is similar in all these cases. (In ref. [8] only a special class of fermion configurations was considered with sign factor $S \equiv 1$, and it was argued that this is enough for lattices strongly asymmetric in the time direction. If, however, not only single pairs of fermion variables are flipped between the timeslices but also touching doublets of pairs, the configurations with negative sign appear. These configurations are not negligible for the time asymmetry factors considered in ref. [8]. I thank Tony Duncan for an illuminating discussion on this.) In the present paper the results for free staggered fermions will be described in the polymer representation where the definition of equivalence classes is simple and which has the advantage of euclidean invariance. (In the case of Wilson fermions in the hamiltonian approach the equivalence classes can also be simply defined, but the restoration of euclidean invariance is a non-trivial requirement [6].)

In order to shortly recapitulate the polymer repre-

sentation of the fermion determinant let us define the free euclidean fermion action in terms of the Grassmann variables ψ_x, $\tilde{\psi}_x$ as

$$S_f = \sum_{xy} \tilde{\psi}_x Q_{xy} \psi_y \equiv \sum_{xy} \tilde{\psi}_x (\delta_{xy} M - K_{xy}) \psi_y. \qquad (10)$$

Here M is the mass parameter and K_{xy} denotes the hopping piece with vanishing diagonal elements. For staggered fermions in four dimensions we have

$$K_{xy} = k \sum_{\mu=1}^{4} (\delta_{x,y+\mu} - \delta_{x+\mu,y})(-1)^{x_1 + x_2 + \dots + x_{\mu-1}}. \qquad (11)$$

The effective hopping parameter is the ratio of k and M: $K \equiv k/M$. The partition function is given by the Grassmann integral

$$Z = \int [\mathrm{d}\psi \, \mathrm{d}\tilde{\psi}] \exp\left(- \sum_{xy} \tilde{\psi}_x Q_{xy} \psi_y \right) = \det Q. \qquad (12)$$

Expanding the exponential in powers of M and K_{xy} it follows from the rules of Grassmann integration, that every non-zero term can uniquely be represented by a "polymer graph" on the lattice: for the mass term proportional to M one has to draw a *monomer* (a single occupied point) and for the products of the hopping terms a set of *polymers* (non-intersecting closed loops of oriented links). Every point on the lattice which is not occupied by a monomer has to be the starting point of an outgoing link and the endpoint of an incoming link. The shortest possible loop is a "dimer" on a single link occupied in both directions. The partition function is the sum over different possible polymer configurations, where the contribution of a configuration is the product of the corresponding M and K_{xy} factors multiplied by an overall negative sign if the number of loops is odd. The expectation values of fermionic variables can be obtained similarly, the only change being the presence of some external monomers or external fermion lines originating at the points where the fermion variables sit [3].

The Monte Carlo procedure on the polymer configurations can be implemented, for instance, by a Metropolis algorithm on plaquettes. The simplest way to store the polymers in the computer is to set up an array jump(site) defined on the lattice points and containing the direction of the link which starts at the

given point. (For the points occupied by a monomer one can take jump = 0.) Sometimes it is useful to also have another array config(link) defined on links and having the value 0 for an unoccupied link, ± 1 for once occupied links (the sign giving the direction), and 2 for doubly occupied links. Considering the information both in jump and config there are altogether 108 possible different states of a plaquette. Uniformly distributed Metropolis proposals for a plaquette change can be taken from a table of size 108·18, because for a given initial state there are either 1, 2, 3 or 9 possible final states. The transition probability on a plaquette is determined by the change of $P \cdot \bar{P}$, where P is given by the number of monomers μ and by the number of polymer links λ as $M^\mu k^\lambda$ and $\bar{P}$ is the absolute value of the average sign factor in the corresponding equivalence class. For the equivalence relation given below by eq. (13) average acceptance rates of about 10% per Metropolis hit can typically be achieved. This relatively low rate is due to the fact that usually a large number of plaquettes cannot be changed at all, because it is blocked by the neighbouring ones. Nevertheless, the autocorrelation times for fermion masses near O(1) are short, typically also of order O(1).

In the case of staggered fermions with hopping matrix in eq. (11) the sign of dimer contributions is positive and also the polymer of length 4 on a plaquette (single plaquette loop) is positive. The shortest negative polymer is a non-planar loop of length 6. The only sign changing transition on a plaquette is the one shown by fig. 1. Therefore, for instance, the polymers built from a tree of parallel lines (see fig. 2) are always positive. These graphs are reminescent of the polymers appearing in QCD in the limit of infinitely strong gauge coupling [9–11].

In order to reduce the sign fluctuations in the expectation value (9) the equivalence classes of poly-
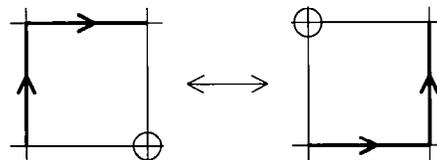

Fig. 1. The only transition on a plaquette which changes the sign of the polymer configuration. The circle denotes a monomer.
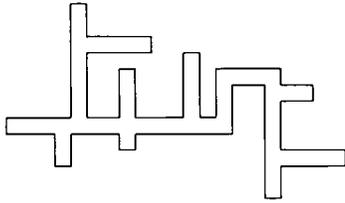
Fig. 2. A polymer built out of a tree of parallel lines which always gives a positive contribution.

mer configurations have to be defined by the sign changing transition in fig. 1. Let us call this transition a *plaquette flip* and denote the flip transformation of the ith plaquette by f_i. If a flip f_i is impossible on a configuration z we put, by definition, $f_i z = 0$. The simplest way to define equivalence classes of configurations is to require that equivalent configurations satisfy

$$z' = f_{i_k} \cdots f_{i_2} f_{i_1} z \,, \tag{13}$$

i.e. z' and z belong to the same equivalence class ($z' \equiv z$) if and only if there exists a sequence of plaquette flips transforming the one into the other. It can be easily seen that this is an equivalence relation, indeed, because from $z_1 \equiv z_2$ it follows $z_2 \equiv z_1$ and if $z_1 \equiv z_2$ and $z_2 \equiv z_3$ then $z_1 \equiv z_3$. By this choice of the equivalence relation the contribution of every polymer configuration is weighted with probabilities which take into account the absolute value of the average sign on the equivalent configurations generated by sequences of plaquette flips. The calculation of the average sign factor is facilitated by a decomposition into clusters.

In order to introduce this cluster decomposition it is useful to consider on a given configuration the set of all *sign changing plaquettes* which can be either directly flipped or can be flipped after flipping other plaquettes. Let us define two flips *connected* if the corresponding transformations are commuting on every configuration. (Commutativity means that the corresponding plaquettes have no common links and no common points changed by the flips.) The maximal sets of connected sign changing plaquettes on a configuration can be called *plaquette clusters*. The importance of plaquette clusters is due to the fact that the sign averages on the equivalence classes of configurations are factorized by them. Namely, if the num-

ber of different configurations of a cluster c with positive sign is $n_+(c)$ and with negative sign $n_-(c)$, then the sign average in the corresponding equivalence class of configurations is

$$\bar{S} = S \prod_c \frac{n_+(c) - n_-(c)}{n_+(c) + n_-(c)} \,. \tag{14}$$

Here S is the sign of the original configuration before any plaquette flip, and the product is performed over the different plaquette clusters. As a simple example, the polymer in fig. 3 defines a four-plaquette cluster with $n_+(c) = 4$ and $n_-(c) = 1$, therefore it contributes to the sign average by a factor $\frac{3}{5}$.

Of course, besides eq. (13) there are also other possibilities for the definition of equivalence classes of polymer configurations. It is possible to restrict the kind of allowed flip sequences in (13). For instance, the size of the cluster to which the flipped sign changing plaquette belongs can be restricted. (Note, that the number of flips cannot directly be restricted in an equivalence relation.) Since the number and length of polymers is unchanged by the flips, one can also restrict the kind of flipped polymers. A more general way of defining equivalence can also allow for the rearrangement of dimers. In this respect it is important to note that dimers are never changed by flip sequences. A simple possibility of this kind is to allow for an arbitrary rearrangement of dimers on a plaquette which can change the sign but is *locked* by a dimer (see fig. 4).

An important property of these equivalence relations is that they are separately defined in regions of the order of the correlation length. Namely, the average size of a sign changing plaquette cluster can be expected to be of the order of the fermion correlation length. (It seems difficult to prove this statement mathematically, but all the numerical experience I obtained up to now is in agreement with this.) This
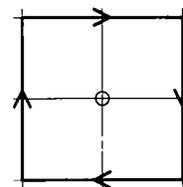

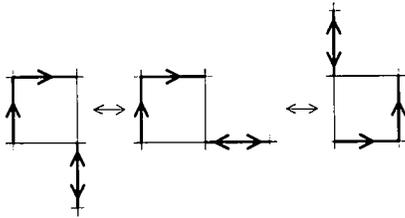Fig. 3. A simple polymer which defines a four-plaquette cluster of sign changing plaquettes.

Fig. 4. Equivalence of configurations by the rearrangement of dimers on a locked sign changing plaquette.

implies that in an updating procedure with the absolute value of the average sign included in the transition probability one can determine the change of the average sign in a region of the order of the correlation length. Therefore, provided that the average sign of the average sign $\langle s(z, U) \rangle$ is near $+1$, for fixed fermion correlation length and for large volumes the computer time needed for this updating procedure grows proportionally to the lattice volume. For decreasing fermion mass (increasing correlation length), however, there is a strong "critical slowing down" because the clusters are growing and becoming more numerous. This critical slowing down depends on the way how the determination of the average sign is implemented. The minimum programming effort is required if the average sign in an equivalence class of configurations is determined by a random walk Monte Carlo process. This goes by choosing plaquettes randomly in a neighbourhood of the updated plaquette and flipping them if possible. If this random walk is sufficiently long every state of the nearby plaquette clusters is reached almost certainly. In this way the plaquettes belonging to nearby clusters can be found and the number of different possible cluster states in eq. (14) can be determined. This gives an exact determination of the change of $\bar{S}$ if every cluster state is reached. The probability of missing some state can be made, in principle, arbitrarily small if the random walk is long enough. Of course, this "Monte Carlo in Monte Carlo" implies an additional critical slowing down which is roughly proportional to the square of the correlated volume, i.e. ξ^8 (besides the usual factor ξ^2 for local updatings). It is also possible to determine the average sign factor on small plaquette clusters exactly by a direct "pattern recognition" method. (For instance, the

configuration in fig. 3 can easily be recognized.) For larger clusters, however, this method becomes very complicated. In any case, for the polymer averaging with the equivalence classes defined above critical slowing down seems to be the main problem. (Let us recall that the required CPU time for the hybrid Monte Carlo algorithm for large volumes (V) and correlation lengths is expected to behave as $V^{5/4}$ $\times \xi^{13/4}$ [14].)

A representative physical quantity which can be easily determined in the polymer representation if $\tilde{\psi}_x \psi_x$. It is related to the number of monomers N_1 by

$$N_1 = am \sum_x \tilde{\psi}_x \psi_x . \tag{15}$$

Here am is the fermion mass in lattice units [in terms of the parameters in the action (10, 11) $am = M/2k$]. The distribution of N_1 can be determined in a way somewhat similar to the procedure applied for the calculation of the density of states [12,13]. Namely, one can consider some interval of the values of N_1 and perform a normal Metropolis Monte Carlo process in it. At every step the value of N_1 is recorded. At the ends of the interval, if a Metropolis change would lead outside of the interval it is never accepted, but the value of N_1 is still recorded. By choosing several partly overlapping intervals it is possible to determine the distribution of N_1 (i.e. the ratios of the expectation values of $\delta_{N_1,N'}$ for different N_1^0) also in a larger range.

The obtained N_1-distribution on a 4^4 lattice for mass $am = 1.0$ is shown by fig. 5. In the present version of the program the average sign in the equivalence classes of configurations is determined exactly for clusters not larger than 2 plaquettes, and randomly for the rest. In addition, rearrangements of dimers on alone standing plaquettes locked by a dimer were also allowed (see fig. 4) if the rearrangement did not interfere with the sign changing flips. The statistics was collected in about 20 000 sweeps in two intervals, namely $82 \leqslant N_1 \leqslant 116$ and $102 \leqslant N_1 \leqslant 128$. These large intervals were possible, because the decomposition of the polymer contributions in eq. (2) was chosen appropriately. Namely, in the positive factor $P(z)$ used in the Monte Carlo updating a somewhat larger mass, actually $am' = 1.25am = 1.25$ was taken. Because of eq. (15) this implies that the decomposition is changed according to
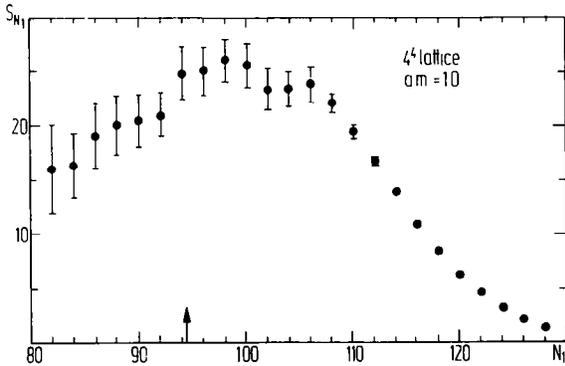
Fig. 5. The distribution of the quantity N_1 defined in eq. (15) for free staggered fermions on a 4^4 lattice at mass $am = 1.0$. The normalization is arbitrary. The arrow shows the correct average value for periodic boundary conditions.

$$R(z) = P'(z)S'(z) , \quad P'(z) = P(z) \cdot 1.25^{N_1(z)} ,$$

$$S'(z) = S(z) \cdot 0.80^{N_1(z)} . \tag{16}$$

Since the plaquette flips do not change N_1, the relation between $s'(z)$ and $s(z)$ is the same as between $S'(z)$ and $S(z)$. The effect of this decomposition is that the statistics over the values of N_1 is distributed more uniformly and, therefore, the intervals can be chosen longer. The obtained N_1 distribution is, of course, independent of the decomposition. This was checked in a control run with the original P. I also performed shorter runs on a 8^4 lattice at $am = 1.0$ and on 4^4 lattice at $am = 0.5$. The former case was unproblematic, but the smaller mass caused a strong slowing down of the program due to an extensive need of random averaging for larger clusters.

Possible lines of improvement are to introduce the exact averaging for larger clusters and/or a different equivalence class definition. Of course, a more important step for the moment is to consider the interactions with bosonic fields, because the optimal equivalence class definition may also depend on the interaction. Due to the problem of critical slowing down it is not clear whether this way of dynamical

fermion simulations is faster than the more conventional methods [1], in the case when these latter are applicable. The main advantage is that polymer averaging or related phase averaging hamiltonian methods are also applicable in cases if the fermion determinant is not positive definite.

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