A Chiral Phase Transition using a
Fermion Cluster Algorithm

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The recent solution to the fermion sign problem allows, for the first time, the use of cluster algorithm techniques to compute certain fermionic path integrals. To illustrate the underlying ideas behind the progress, a cluster algorithm is constructed to study the chiral phase transition in a strongly interacting staggered fermion model with an arbitrary mass term in $3 + 1$ dimensions. Unlike conventional methods there is no difficulty in the cluster method to approach the chiral (massless) limit. Results using the new algorithm confirm that the chiral transition falls under the expected universality class.

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I. Introduction

The past few years has been a time of remarkable progress in our understanding of lattice fermions and their ability to reproduce the chiral properties of the continuum theory. It is now possible to formulate vector-like gauge theories on the lattice with all its chiral symmetry intact. Our understanding of non-perturbative formulations of chiral gauge theories is also advancing at a remarkable rate as is reflected by many recent contributions. On the other hand, our ability to perform reliable (numerical) calculations in many theories involving strongly interacting fermions and especially in the chiral limit has remained primitive. In particular algorithms based on hybrid molecular dynamics, that are popular for gauge theories like QCD, suffer either from sign problems or critical slowing down in the chiral limit. Unless better numerical methods are found, it is likely that we will be forced to perform most of our calculations far from the chiral limit and hence not gain from the progress in our understanding of chiral symmetry.

Numerical methods for fermionic systems are especially difficult due to the Pauli-exclusion principle. The Boltzmann weight of the statistical mechanics problem describing such systems can often become negative thereby invalidating most Monte-Carlo methods. This is usually referred to as the sign problem. In other cases one is often forced to work with bosonic variables with non-local Boltzmann weights which arise through the
fermion determinant. Such expressions are not easy to handle and there is no known way to overcome problems like critical slowing.

Recently a new numerical method to perform fermionic path integrals has emerged and is based on a rather novel form of bosonization. Instead of the Grassmann variables, the method starts by representing fermions through their occupation numbers. Such representations, which have been studied in the past [4, 5], were not considered useful due to sign problems. Over the past year it has become clear that at least in a class of models it is possible to design cluster algorithms which automatically solve the fermion sign problem and provide an alternative way to compute fermionic path integrals. In a sense the algorithm suggests a new way to bosonize the model in terms of dynamics of clusters. The new method works in both relativistic [6, 7] and non-relativistic [8] models. Since cluster algorithms are known to beat critical slowing down in a variety of bosonic models [9, 10], the new algorithms have the ability to work efficiently even in the presence of long correlation lengths. In particular, they encounter no difficulties in the limit where the fermions become massless.

The present article illustrates the main features of the new approach through an example of a four Fermi model involving staggered fermions. This model undergoes a $Z_2$ chiral transition from a high temperature chirally symmetric phase to the broken phase at low temperatures and was studied originally in the chiral limit in [7]. Here the earlier work is extended to include a fermion mass. This extension turns out to be quite useful because on a large but finite lattice all the interesting properties of the chiral condensate, as an order parameter of the transition, emerge only when a tiny mass can be added to the system. In the next section the partition function of the model is written in the occupation number basis and the origin of the fermion sign problem is reviewed. In section 3 the partition function is rewritten in terms of connected fermion world-line configurations that arise due to the introduction of local "bond" variables. In the new variables the solution to the sign problem emerges naturally and leads to a very elegant cluster algorithm. In section 4, the algorithm and some numerical results are discussed. Section 5 contains conclusions along with a description of on-going work and points to new directions for the future.

II. The Model

The model considered in this article involves interacting staggered fermions hopping on a 3-d cubic spatial lattice with $V = L^3$ sites $x$ ($L$ even) and with anti-periodic spatial boundary conditions. The dynamics of the fermions is described through the Hamilton
operator
\[ H = \sum_{x,i} h_{x,i} + m \sum_x p_x \]  
(1)

where the term
\[ h_{x,i} = \frac{1}{2} \eta_{x,i} \left( \Psi^+_x \Psi_{x+i} + \Psi^+_{x+i} \Psi_x \right) + (\Psi^+_x \Psi_x - \frac{1}{2})(\Psi^+_{x+i} \Psi_{x+i} - \frac{1}{2}), \]  
(2)
couples the fermion operators at the lattice sites \( x \) and \( x + \hat{i} \), where \( \hat{i} \) is a unit-vector in the \( i \)-direction and the mass term
\[ p_x = (-1)^{x_1+x_2+x_3}(\Psi^+_x \Psi_x - 1/2), \]  
(3)
is a single site operator. The fermion creation and annihilation operators \( \Psi^+_x \) and \( \Psi_x \) used in the above equations satisfy the standard anti-commutation relations
\[ \left\{ \Psi^+_x, \Psi_y \right\} = \left\{ \Psi_x, \Psi^+_y \right\} = 0, \left\{ \Psi^+_x, \Psi_y \right\} = \delta_{xy}. \]  
(4)
Further \( \eta_{x,1} = 1, \eta_{x,2} = (-1)^{x_1} \) and \( \eta_{x,3} = (-1)^{x_1+x_2} \) are the standard staggered fermion sign factors. In the chiral limit \( (m = 0) \), the above Hamiltonian was discussed in [7].

In addition to the usual \( U(1) \) fermion number symmetry, there are a number of discrete symmetries of the staggered fermion Hamiltonian as discussed in [11]. For example, at \( m = 0 \) the Hamiltonian is invariant under shifts of \( \Psi^+_x \) and \( \Psi_x \) by one lattice spacing in the \( x_3 \) direction. The mass term breaks this \( \mathbb{Z}_2 \) symmetry which is known to be a subgroup of the well known chiral symmetry of relativistic massless fermions. Here this symmetry is broken spontaneously at low temperatures while thermal fluctuations restore it at high temperatures. The associated second order phase transition belongs to the universality class of the 3d ising model as discussed in [7]. The extension discussed here, allows one to add a tiny mass and hence study the transition using the chiral condensate.

In order to construct the path integral representation of the partition function the Hamilton operator is first decomposed into seven terms \( H = H_1 + H_2 + \ldots + H_6 + H_7 \) with
\[ H_i = \sum_{x=(x_1,x_2,x_3)} h_{x,i} \text{ for } i = 1, 2, 3; \quad H_7 = m \sum_x p_x. \]  
(5)

This decomposition is exactly the same as the one used in [7] for the \( m = 0 \) case, where \( H_7 \) was absent. The various steps in the construction of the partition function from here on is exactly the same as in [7]. Leaving the details to that paper only the essential points are sketched here. The Suzuki-Trotter formula leads to the expression
\[ Z_f = \text{Tr}[\exp(-\beta H)] = \lim_{M \to \infty} \text{Tr}[e^{-\epsilon H_1}e^{-\epsilon H_7/6}\ldots e^{-\epsilon H_6}e^{-\epsilon H_7/6}]^M, \]  
(6)
for the fermionic partition function at inverse temperature $\beta$, where $\epsilon = \beta/M$ is the lattice spacing in the Euclidean time direction. Spreading $H_7$ symmetrically with each $H_i, i = 1, \ldots, 6$ is not necessary except that it adds some symmetry to the algorithm. Further, in the arguments given below, $M$ is assumed to be finite and that the true partition function is obtained from an extrapolation of the data obtained from a series of simulations at larger and larger $M$. Fortunately it is also possible to formulate the cluster algorithm in the time continuum limit as demonstrated in [12].

![Diagram of a fermion world-line configuration with $\text{Sign}_t[n] = -1$ on a one dimensional periodic spatial lattice of size $L = 8$ where the time slice $t = 3\epsilon$ is the same as $t = 0$.](image)

**FIG. 1.** A fermion world-line configuration with $\text{Sign}_t[n] = -1$ on a one dimensional periodic spatial lattice of size $L = 8$ where the time slice $t = 3\epsilon$ is the same as $t = 0$.

It is well known that in the occupation number basis a fermionic partition function can be written as a sum over fermion world-line configurations[4]. Since the fermionic creation operators anti-commute, the information that a subset of the lattice sites are occupied defines the state of the system only up to a sign. A complete definition of the occupation number basis states requires an ordering of the entire lattice which then specifies the order in which the fermions on the lattice are created. Taking this ordering into account it is possible to write the partition function as a sum over configurations of fermion occupation numbers $n(x, t) = 0, 1$ on a $(3+1)$-d space-time lattice of points $(x, t)$ where $t = \epsilon n/12, n = 0, 1, 2, \ldots (12M - 1)$ labels the time slices. The trace imposes the periodicity constraint $n(x, 0) = n(x, \beta)$. A typical configuration in one spatial dimension
is shown in figure 1, where the shaded regions depict either a two site interaction due to \( \exp(-h_{x,i}) \) or a single site interaction due to \( \exp(-mp_x) \).

The Boltzmann weight of each configuration \( n \) is a product of transfer matrix elements associated with the configuration of fermions on each shaded region. These elements are shown in figure 2. Representing the magnitude of the Boltzmann weight by \( W[n] \) and

Non-zero elements due to \( \exp(-h_{x,i}) \) \hspace{1cm} \text{Non-zero elements due to } \exp(-p_x) 

(a) \hspace{1cm} (b) 

(c) \hspace{1cm} (d) 

(e) \hspace{1cm} (f) 

(g) \hspace{1cm} (h) \hspace{1cm} (i) \hspace{1cm} (j) 

even site \hspace{1cm} odd site

FIG. 2. The figures (a) through (j) illustrate the non-zero transfer matrix elements. Weight of (a),(b) is \( \exp(-\epsilon/4) \); weight of (c),(d) is \( \exp(\epsilon/4) \cosh(\epsilon/2) \); weight of (e),(f) is \( \Sigma \exp(\epsilon/4) \sinh(\epsilon/2) \); weight of (g),(j) is \( \exp(-m\epsilon/12) \) and weight of (h),(i) is \( \exp(m\epsilon/12) \). The factor \( \Sigma \) is a product of local sign factors \( \eta_{x,i} \) and non-local sign factors that arise due to anti-commutation relations. Further, \( x_1 + x_2 + x_3 = \text{even(odd)} \) defines an even(odd) site.

the sign, which takes into account the various anti-commutation relations, by \( \text{Sign}[n] \) the partition function takes the form

\[
Z_f = \sum_n \text{Sign}[n] W[n]. \tag{7}
\]

Clearly \( \text{Sign}[n] \) is the product of the sign factors \( \Sigma \) that appear in the transfer matrix elements associated to fermion hops represented through figures 2(e) and 2(f). When the fermion hops from \( x \) to \( x + \hat{i} \) or vice versa due to the action of \( \exp(-h_{x,i}) \) it picks up a product of local sign factors due to terms like \( \eta_{x,i} \) as well as a string of non-local signs that arise due to anti-commutation relations involved when the fermion has to cross other fermions on the ordered lattice while reaching its destination. The evaluation of this non-local part of \( \Sigma \) is rather tedious. Separating the two parts, one can define \( \text{Sign}[n] = \text{Sign}_f[n] \text{Sign}_b[n] \), where \( \text{Sign}_f[n] \) comes from the product of non-local parts of \( \Sigma \)
and is purely fermionic, where as Sign_{b}[n] is the one that comes from the local parts and may arise even in bosonic models. Fortunately Sign_{f}[n] has a topological meaning. The occupied lattice sites define fermion world-lines which are closed around the Euclidean time direction. However, during their Euclidean time evolution fermions can interchange their positions, and the fermion world-lines thus define a permutation of particles. The Pauli exclusion principle dictates that the Sign_{f}[n] is just the sign of that permutation. Further, Sign_{b}[n] receives an extra minus-sign for every fermion that hops across a spatial boundary due to anti-periodic boundary conditions.

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FIG. 3. The figure on the left shows a connected fermion world-line configuration in one space and one time dimension. The figure on the right is obtained after flipping a cluster (which is shown) from the configuration on the left. The resulting new connected fermion world-line configuration is the “reference” configuration of the model.

III. Bond Variables and Meron Clusters

When the partition function is written as a sum over fermion world-line configurations, the Boltzmann weight of each configuration is not guaranteed to be positive definite. This leads to the well known fermion sign problem. It was discovered recently that sometimes it is possible to solve this problem when the Boltzmann weight of each fermion world line configuration is written as a sum of Boltzmann weights describing new type of configurations, referred to as “connected” fermion world line configurations, obtained by the introduction of bond variables that establish connections with in the lattice. An example of this new type of configuration is shown in figure 3. In a class of models,
FIG. 4. The figure shows how to rewrite the weight of each configuration of figure 2 in terms of new configurations that have bonds in addition to fermions.
including the one considered in this article, it is possible to regroup these new type of configurations such that the sum of the weights of each group is positive or zero, thus canceling all negative weights. The regrouping is accomplished by identifying all possible connected fermion world-line configurations obtained by flipping clusters of connected lattice sites. By flipping a lattice site one means that if the site is filled (with a fermion) it is emptied and vice versa. The result of a cluster flip is also shown in Figure 3.

In order to calculate the Boltzmann weight of every new type of configurations each interaction plaquette of in the old configuration given in figure 2 is rewritten as a sum of new configurations that involve bonds in addition to the fermions. The sign factors $\Sigma$ are ignored at this step and will be considered during the regrouping step. Further, the bonds are introduced so that they obey the property of a flip symmetry. This means that the magnitude of the Boltzmann weight of connected fermions world line configurations do not change when connected sites are flipped. This property will be useful to identify configurations with equal weight but opposite signs during the regrouping step. For the two site interactions the weights of the new bond variables is shown at the top of figure 4. For the single site interaction due to the mass terms one has to distinguish between even and the odd sites since the weights differ on these two sites. However, now by introducing two types of bonds the property of flip symmetry can be maintained as shown in the bottom part of figure 4. The difference between the two bonds is that when the sites connected by the “dashed” bond are flipped, an extra sign change has to be taken into account. These signs must be multiplied to the $\text{Sign}[n]$ and the overall sign should be taken into account at the regrouping stage.

The above procedure gives a new expression for the path integral in terms of connected fermion world-line configurations.

$$Z_f = \sum_c \text{Sign}[C] \ W[C]$$ (8)

Each configuration $C$ now defines a set of clusters in addition to the fermion occupation numbers as shown in figure 3. For the present model the clusters form closed loops. The weight $W[C]$ of each configuration can be read off using the rules of figure 4. The $\text{Sign}[C]$ is the product of $\text{Sign}[n]$ for the old configuration obtained by ignoring the bond and the extra negative sign factors that may arise from filled dashed-bonds on even sites and empty dashed-bonds on odd sites. A great simplification occurs when the flip symmetry imposed during the bond introduction is used. If a configuration $C$ has $N_c$ clusters, then all the $2^{N_c}$ configurations, obtained by flipping the clusters independently, have the same weight $W[C]$. This degeneracy can be used to regroup the configurations and write

$$Z_f = \sum_c \text{Sign}[C] \ W[C]$$ (9)
where $\bar{\text{Sign}[C]}$ is the average of $\text{Sign}[C]$ over these $2^{N_C}$ configurations. The usefulness of eq. (9) can be appreciated when $\text{Sign}[C]$ obeys the following two properties:

1. $\text{Sign}[C] = \prod_{i=1}^{N_C} \text{Sign}[c_i]$, where $\text{Sign}[c_i]$ is the sign of the $i$th cluster configuration labeled $c_i$.

2. For every configuration the individual clusters can be flipped to a reference configuration $c_i^{\text{ref}}$ such that $\text{Sign}[c_i^{\text{ref}}] = 1$.

It is then easy to show that $\bar{\text{Sign}[C]} = 0$, if there is at least a single cluster whose flip changes the sign of the configuration, i.e., there is a cluster $c_i$ such that $\text{Sign}[c_i^{\text{non-ref}}] = -1$. Such clusters are referred to as merons. A configuration with no merons will then have $\bar{\text{Sign}[C]} = 1$. There are models in which $\text{Sign}[C]$ has the above two properties and the present model falls in this class. Although the first property of $\text{Sign}[C]$ is difficult to establish, it is easy to show that every cluster in the present model can always be flipped such that all even sites are empty and odd sites are filled in the present model. This leads to the staggered configuration shown on the right in figure 3.

The new expression for the partition function derived in eq. (9) shows that fermion dynamics in the present model is equivalent to a statistical mechanics of clusters. Each cluster has two degrees of freedom related to the fermions. The Pauli-exclusion principle is encoded in the fact that meron clusters contribute zero weight to the partition function. In order to determine if a cluster is a meron or not, one has to understand its topology. If $n_h$ is the number of hops of the cluster to the neighboring lattice site on the same time slice, $n_\eta$ is the number of local signs that the cluster encounters during the hops, $n_w$ is the temporal winding and $n_d$ is the number of dashed bonds in the cluster, then the cluster is a meron if $(n_w + n_h/2 + n_d + n_\eta)$ is an even integer. Cluster algorithms based on the concept of merons was originally invented in [13] and are referred to as the meron cluster algorithms.

IV. Algorithm and Results

It is easy to construct cluster algorithms that generate clusters with weight $W[C]$ obtained using the rules given in figure 4. This makes it possible to simulate the modified model obtained by ignoring the sign factors. The partition function of the resulting model, denoted by $Z_b$, can be expressed as a sum over contributions from various meron sectors, i.e., $Z_b = \sum_N Z_N$ where $N$ denotes the number of merons in a cluster configuration. On the other hand the actual partition function $Z_f = Z_0$. Since a typical configuration of $Z_b$ is filled with merons, it is exponentially difficult to find zero meron sectors and the cluster algorithm is still inefficient for simulating the dynamics of $Z_f$. A solution to the
problem of avoiding configurations with meron clusters is necessary. Fortunately, using a local Metropolis accept-reject step, it is possible to introduce a re-weighting factor that suppresses higher meron sectors. For example the Metropolis step can modify the weight of cluster configurations to \( W[C]/p^N \), where \( p > 1 \) and \( N \) represents the number of merons in the configuration. This modifies \( Z_b \) but leaves \( Z_f \) unchanged! This Metropolis step then increases the efficiency of the algorithm by an exponential factor.

A variety of quantities can be calculated with the new algorithm. The first step, however, is to find expressions for these quantities in terms of cluster variables. Operators that are diagonal in the occupation number basis are easy to calculate, although more general operators can also be evaluated. For some quantities it is possible to find analytic expressions for the average over all the cluster flips, which are referred to as improved estimators. The chiral condensate in the present problem, which is also the order parameter for the chiral phase transition, is one such quantity. In the operator language the condensate is defined as

\[
\langle \bar{\psi} \psi \rangle = \frac{1}{V} \frac{\text{Tr}[e^{-\beta H} O]}{\text{Tr}[e^{-\beta H}]},
\]

where \( O = \sum_x p_x \). The improved estimator on the other hand is given by

\[
\langle \bar{\psi} \psi \rangle = \frac{1}{2} \frac{\langle p \text{ Size}(c_{\text{meron}}) \delta_{N,1} \rangle}{\langle \delta_{N,0} \rangle V \beta},
\]

where \( \langle \delta_{N,0} \rangle \) represents the mean number of empty sites in the configuration.
where \( N \) is the number of merons in the cluster configuration generated by the algorithm and \( \text{Size}(c_{\text{meron}}) \) is the size of the meron cluster. The extra re-weighting factor \( p \) takes into account the modifications due to the Metropolis step. It is easy to show that on a finite lattice in the \( m = 0 \) limit there are no single meron sectors and hence the chiral condensate simply vanishes. On the other hand, as seen in figure 5, an extremely tiny mass \( m = 0.001 \) shows convincingly the effects of spontaneous symmetry breaking. The critical value of \( \beta_c = 0.948 \) obtained through finite size scaling analysis in [7] appears consistent with the present results. In [8] the chiral susceptibility was measured in the chiral limit its behavior near the transition was shown to be consistent with the universality class of the 3-d ising model. A more detailed analysis of the data from the present study will be presented elsewhere.

V. Conclusions

The fermion cluster algorithm constructed in this article is an example of a novel way to compute fermionic path integrals. The sign problems that arise in the new method are solved using the concept of a meron which makes it easy to match all the configurations with negative Boltzmann weight with configurations with an equal but positive Boltzmann weight. Some interesting features emerge with the new algorithm. For the first time it is possible to treat fermions and bosons on an equal footing in simulations[1-4]. Further it is possible to approach chiral limits more easily as discussed here.

A number of applications of the new techniques are presently being studied. For example it appears possible to find models with continuous chiral symmetry in which the sign problem can be completely solved. Chiral symmetry breaking in such a system will lead to the existence of massless Goldstone particles in the chiral limit. Apart from clarifying issues of universality the presence of the low mass particles can help in studying resonance physics that become difficult with conventional algorithms. Applications to non-relativistic many fermion problems is another topic where the present techniques are directly applicable. It is also likely that solutions to Hubbard type models will emerge with these techniques.

Adding gauge fields introduces new negative signs. It will be exciting to find solutions to this class of sign problems using cluster methods. There is evidence from strong coupling limits that a regrouping of configurations that differ in both gauge and fermion content can help solve such problems. This question is presently under investigation.
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