Meron-cluster algorithms and chiral symmetry breaking in a (2 + 1)-d staggered fermion model *

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MIT-CTP 2965, BUTP-2000-08

October 28, 2018

Abstract

The recently developed Meron-Cluster algorithm completely solves the exponentially difficult sign problem for a number of models previously inaccessible to numerical simulation. We use this algorithm in a high-precision study of a model of $N = 1$ flavor of staggered fermions in (2+1)-dimensions with a four-fermion interaction. This model cannot be explored using standard algorithms. We find that the $\mathbf{Z}(2)$ chiral symmetry of this model is spontaneously broken at low temperatures and that the finite-temperature chiral phase transition is in the universality class of the 2-d Ising model, as expected.

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*This work is supported in part by funds provided by the U.S. Department of Energy (D.O.E.) under cooperative research agreement DE-FC02-94ER40818 and by the Schweizerischer Nationalfonds.
1 Introduction

There are a number of models of interest which suffer from a very severe sign problem. This includes QCD and other field theories with a non-zero chemical potential or a non-zero vacuum angle or odd numbers of fermion flavors, frustrated quantum spin systems, like the quantum antiferromagnet in an external magnetic field, and models for strongly-correlated electrons, like the Hubbard model for high-temperature superconductivity. These models have a Boltzmann weight which can be negative or even complex and so cannot be interpreted as a probability. This difficulty can be overcome in numerical simulations by including the sign or phase of the Boltzmann weight with observables. Unfortunately, this leads to large cancellations and gives exponentially small observables. This requires exponentially large statistics, which makes it in practice impossible to simulate these models numerically.

Recently, a new technique has been developed, called Meron-Cluster algorithms [1], which completely solves the sign problem for some of these models [2, 3]. It identifies the origin of the sign problem with properties of the clusters, which enables it to be eliminated. Cluster algorithms in general are extremely efficient at exploring configuration spaces and very often do not suffer from critical slowing down as a phase transition is approached, unlike many other algorithms. For example, in this and previous papers, we can work directly in the chiral limit with massless fermions. Combined with the ability to construct improved estimators, we can perform a high precision study of these models with only modest statistics.

In this paper, we explore a model of $N = 1$ flavor of staggered fermions in (2+1)-dimensions with a four-fermion interaction. This model has a very severe sign problem and cannot be simulated with standard techniques. We build a Meron-Cluster algorithm, which we use to perform a high-precision study. We find that the $\mathbb{Z}(2)$ chiral symmetry of this model is spontaneously broken at low temperatures and, using finite-size scaling analysis, we verify that the finite-temperature chiral phase transition is in the universality class of the 2-d Ising model. A recent study of the same model with $\mathbb{Z}(2)$ chiral symmetry in (3+1)-dimensions has shown, using a Meron-Cluster algorithm, that a finite temperature chiral phase transition occurs which has the universal behavior of the 3-d Ising model [4]. The work presented in this paper concerns a different universality class and also constructs more observables than were previously considered.

The identification of the finite temperature critical behavior is not entirely straightforward [4]. A model of $N$ fermion flavors with a four-fermion interaction shows mean-field behavior in the $N = \infty$ limit. On the other hand, at finite $N$ one finds the non-trivial critical behavior that one expects based on dimensional reduction and standard universality arguments. For example, in [4] it has been verified that the chiral phase transition in a (2+1)-d four-fermion interaction model with $N = 4$
flavors and \( \mathbb{Z}(2) \) chiral symmetry is in the universality class of the 2-d Ising model. Due to the fermion sign problem, standard fermion simulation methods often do not work in models with too small a number of flavors. The work presented in this paper shows that the same universal behavior holds for \( \mathcal{N} = 1 \) flavor.

The standard technique to deal with fermions in Monte-Carlo simulations is to integrate them out, resulting in a non-local bosonic theory. The Meron-Cluster algorithm does not integrate out the fermions, instead we describe them with a local theory using a Fock space basis of occupation number. The fermion sign arises as a non-local property due to the permutation of fermion world lines. Using probabilistic rules, we connect neighboring lattice sites, producing closed loops, which are the clusters. A cluster is flipped by making all of its occupied sites empty and its empty ones occupied. Such a cluster flip can change the fermion sign by changing the permutation of fermion world lines. A cluster whose flip changes the sign we call a meron. We can tell if a cluster is a meron simply from its structure. A typical configuration contains many merons, yet the observables of interest are only non-zero for configurations with very few or no merons. The signals from standard Monte Carlo algorithms are so exponentially small because the Markov chain explores a vast configuration space, yet only an exponentially small sub-space makes any contribution to measurables. By restricting ourselves to only explore the relevant sub-space, we completely solve the sign problem.

This paper is organized as follows. In section 2, we present the fermionic model which we have studied, calculate its partition function using the Hamiltonian formulation and find that there is a sign problem. In section 3, we describe briefly the Meron-Cluster algorithm which we have used to perform numerical simulations of this model. We present the results of the simulations in section 4 and give our conclusions in section 5.

2 The Staggered Fermion Model

We consider staggered fermions in the Hamiltonian formulation on a 2-dimensional spatial lattice of extent \( L \), which is even. The Hamiltonian operator is

\[
H = \sum_{x,i} h_{x,i} + m \sum_x (-1)^{x_1 + x_2} \Psi_x^+ \Psi_x
\]

\[
h_{x,i} = \eta_{x,i}(\Psi_x^+ \Psi_{x+i} + \Psi_{x+i}^+ \Psi_x) + G(\Psi_x^+ \Psi_x - \frac{1}{2})(\Psi_{x+i}^+ \Psi_{x+i} - \frac{1}{2}),
\]

where \( \eta_{x,1} = 1 \) and \( \eta_{x,2} = (-1)^{x_1} \) are the standard Kawamoto-Smit phases for staggered fermions and \( G \) is a constant. The fermionic operators satisfy the usual anticommutation relations \( \{\Psi_x, \Psi_y\} = \{\Psi_x^+, \Psi_y^+\} = 0, \{\Psi_x^+, \Psi_y\} = \delta_{xy} \). The same model in \((3+1)\)-dimensions was explored in [2]. We refer the reader to this paper,
where various features of the model and the Meron-Cluster algorithm are discussed in more detail than we give here.

In the Hamiltonian formulation of the theory, fermion doubling on the lattice occurs only in the spatial dimensions. Using staggered fermions, the Dirac components of a spinor are distributed spatially, reducing the number of fermion flavors by a factor of four. Thus this (2+1)-dimensional model contains $N = 1$ fermion flavor. The model has a global $U(1)$ symmetry corresponding to conserved particle number, as the total particle number operator commutes with the Hamiltonian

$$N = \sum_x \Psi_x^+ \Psi_x, \quad [H, N] = 0. \quad (2.2)$$

Furthermore the Hamiltonian has, for $m = 0$, a discrete $\mathbb{Z}(2)$ symmetry corresponding to shifts by one lattice spacing. However the mass term breaks that symmetry explicitly. For a single flavor of massless fermions, the symmetry of the lattice model is $U(1) \otimes \mathbb{Z}(2)$ and we refer to the discrete symmetry as chiral symmetry. In the continuum, a single massless fermion flavor has a $U(1)$ axial symmetry (there is no gauge interaction, so this symmetry is not anomalously broken). The discrete $\mathbb{Z}(2)$ symmetry is the lattice remnant of this continuous symmetry. From now on, we set $m = 0$ and explore the behavior of the chiral symmetry of this model. The symmetries of staggered fermions are discussed in detail in Ref. [6]. If the $\mathbb{Z}(2)$ chiral symmetry is spontaneously broken at some finite temperature, from universality we expect this to be a second-order phase transition. As the critical point is approached, the correlation length $\xi$ diverges and the system becomes insensitive to the time extent. Due to dimensional reduction, we expect a finite-temperature chiral phase transition in this model to belong to the 2-d Ising universality class.

The partition function of the model is

$$Z = \text{Tr}[\exp(-\beta H)] = \lim_{M \to \infty} \text{Tr}[\exp(-\epsilon H)]^M \quad (2.3)$$

$$= \lim_{M \to \infty} \text{Tr}[\exp(-\epsilon H_1) \exp(-\epsilon H_2) \exp(-\epsilon H_3) \exp(-\epsilon H_4)]^M,$$

where we use the Suzuki-Trotter decomposition to divide the Euclidean time extent $\beta$ into $4M$ time slices, the lattice spacing in the time direction being $\epsilon = \beta/M$. The Hamiltonian operator is decomposed into four parts $H = H_1 + H_2 + H_3 + H_4$. All of the terms that contribute to a particular $H_i$ commute with one another, as each term is an interaction between nearest-neighbors and each lattice site appears in only one such nearest-neighbor pair. However, the $H_i$ do not commute with one another. We note that it is not actually necessary to discretize the time direction, as it is possible to work directly in the Euclidean time continuum [7].

We can equivalently describe this model with bosonic operators, using a transformation by Jordan and Wigner [8]. We order the lattice sites on each time slice arbitrarily into a chain, which can be done in any number of spatial dimensions. For example, a possible ordering of points in two spatial dimensions is by an index
\( l = x_1 + (x_2 - 1)L \). The fermionic operators are now represented by a chain of Pauli matrices

\[
\Psi_x^+ = \sigma_1^3 \sigma_2^3 \ldots \sigma_{l-1}^3 \sigma_l^+, \quad \Psi_x = \sigma_1^3 \sigma_2^3 \ldots \sigma_{l-1}^3 \sigma_l^-,
\]

\[
\Psi_x^+ \Psi_x = \frac{1}{2} (\sigma_l^3 + 1)
\]

(2.4)

\[
\sigma^\pm = \frac{1}{2} (\sigma^1 \pm i\sigma^2), \quad [\sigma_i^j, \sigma_m^j] = 2i\delta_{lm} \epsilon^{ijk} \sigma_k^j,
\]

where the spatial position \( x \) is denoted by the index \( l \) and the Pauli matrices satisfy the usual commutation relations. To calculate the partition function of the theory, we use the Fock space basis of occupation number \( n_x = 0, 1 \) i.e. the eigenstates of \( \sigma^3 \). The occupied and empty states are respectively \( |1\rangle \) and \( |0\rangle \), which satisfy \( \sigma^3 |1\rangle = |1\rangle \) and \( \sigma^3 |0\rangle = -|0\rangle \).

The time evolution operator \( \exp(-\epsilon H_x) \) acts on a time slice of occupation number states, producing the next time slice. This is decomposed into the product of operators \( \exp(-\epsilon h_{x,i}) \) acting on nearest-neighbor occupation states. The transfer matrix is

\[
\exp(-\epsilon h_{x,i}) = \exp\left(\frac{\epsilon G}{4} \begin{pmatrix} 0 & 0 & 0 & 0 \\ \cosh \frac{\epsilon}{2} & \Sigma \sinh \frac{\epsilon}{2} & 0 & 0 \\ 0 & \Sigma \sinh \frac{\epsilon}{2} & \cosh \frac{\epsilon}{2} & 0 \\ 0 & 0 & 0 & \exp(-\frac{\epsilon G}{2}) \end{pmatrix} \right),
\]

(2.5)

the basis being \( |00\rangle, |01\rangle, |10\rangle \) and \( |11\rangle \), where e.g. \( |01\rangle \) represents state \( |0\rangle \) at \( x \) and \( |1\rangle \) at \( x + i \). If these nearest-neighbors are labelled \( l \) and \( m \), the off-diagonal transfer matrix elements have a factor \( \Sigma = \eta_{x,i} \sigma_{l+1}^3 \sigma_{l+2}^3 \ldots \sigma_{m-1}^3 \). Note that this operator is diagonal in the occupation number basis.

The partition function of the theory is given as a path integral

\[
Z_f = \sum_n \text{Sign}[n] \exp(-S[n]),
\]

(2.6)

where we sum over all possible configurations of occupation numbers \( n(x,t) = 0, 1 \) on a \((2+1)\)-d space-time lattice of points \((x,t)\). The Boltzmann factor \( \exp(-S[n]) \) for a configuration is the product of the Boltzmann factors for each space-time plaquette \( \exp(-s[n(x,t), n(x+i,t), n(x,t+1), n(x+i,t+1)]) \), which are

\[
\exp(-s[0,0,0,0]) = \exp(-s[1,1,1,1]) = \exp(-\frac{\epsilon G}{2}),
\]

\[
\exp(-s[0,1,0,1]) = \exp(-s[1,0,1,0]) = \cosh \frac{\epsilon}{2},
\]

\[
\exp(-s[0,1,1,0]) = \exp(-s[1,0,0,1]) = \sinh \frac{\epsilon}{2}.
\]

(2.7)

All other plaquettes are illegal and have Boltzmann weight zero, as they represent non-conservation of fermion number. Any configuration which contains illegal
plaquettes has itself Boltzmann weight zero and makes no contribution to the partition function. We are only interested in legal configurations, which have to satisfy several constraints. Note that here we have dropped the overall factor $\exp(eG/4)$ that appeared in eq. (2.3). The sign of a configuration, $\text{Sign}[n]$, is also a product of space-time plaquette contributions $\text{sign}[n(x, t), n(x + \hat{i}, t), n(x, t + 1), n(x + \hat{i}, t + 1)]$ with

$$
\text{sign}[0, 0, 0, 0] = \text{sign}[0, 1, 0, 1] = \text{sign}[1, 0, 1, 0] = \text{sign}[1, 1, 1, 1] = 1, \\
\text{sign}[0, 1, 1, 0] = \text{sign}[1, 0, 0, 1] = \Sigma.
$$

(2.8)

The occupied lattice sites define world-lines of fermions, which close due to the periodicity of the Euclidean time direction. The world-lines are free to permute during their time evolution as the fermions interchange position and each configuration has a well-defined permutation of fermions. The Pauli exclusion principle tells us that the sign of a configuration is the permutation sign of the fermions, hence $\text{Sign}[n] = \pm 1$. This non-local effect is contained in the factors $\Sigma$ of each space-time plaquette.

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The expectation value of a fermionic observable $A[n]$ is given by

$$
\langle A \rangle_f = \frac{1}{Z_f} \sum_n A[n] \text{Sign}[n] \exp(-S[n]) = \frac{\langle A \text{Sign} \rangle}{\langle \text{Sign} \rangle},
$$

(2.9)

$$
\langle \text{Sign} \rangle = \frac{1}{Z_b} \sum_n \text{Sign}[n] \exp(-S[n]),
$$

where $\langle ... \rangle$ means a measurement made in the bosonic ensemble, whose partition function is $Z_b = \sum_n \exp(-S[n])$. To measure one fermionic observable requires two bosonic measurements. The quantities of physical interest which we measure are the chiral condensate $\bar{\Psi}\Psi$, the chiral susceptibility $\chi$ and a Binder cumulant $U$ of the chiral condensate, respectively

$$
\bar{\Psi}\Psi[n] = \frac{e}{4} \sum_{x,t} (-1)^{x_1 + x_2} (n(x, t) - \frac{1}{2}),
$$

$$
\chi = \frac{1}{\beta V} \langle (\bar{\Psi}\Psi)^2 \rangle_f, \quad U = 1 - \frac{\langle (\bar{\Psi}\Psi)^4 \rangle_f}{3\langle (\bar{\Psi}\Psi)^2 \rangle_f^2},
$$

(2.10)

3 The Meron-Cluster Algorithm

We now describe briefly the Meron-Cluster algorithm which we used to sample the bosonic ensemble corresponding to the fermionic model without the sign factor. We set $G = 1$, for which the bosonic model is the isotropic antiferromagnetic quantum Heisenberg model, whose Hamiltonian is $H = \sum_{x,i} (S^1_x S^1_{x+i} + S^2_x S^2_{x+i} + S^3_x S^3_{x+i})$, where $S^l_x = \frac{1}{2}\sigma^l_x$ is a spin 1/2 operator at the lattice site $x$, labelled by $l$ in the Jordan-Wigner chain. There already exist extremely efficient cluster algorithms to simulate
weight & configuration & break-ups \\
--- & --- & --- \\
exp \left( -\frac{\epsilon}{2} \right) & ![Diagram of a configuration] & ![Diagram of break-ups] \\
\cosh \left( \frac{\epsilon}{2} \right) & ![Diagram of a configuration] & ![Diagram of break-ups] \\
\sinh \left( \frac{\epsilon}{2} \right) & ![Diagram of a configuration] & ![Diagram of break-ups] \\

Table 1: Cluster break-ups of various plaquette configurations together with their probabilities, where \( p = \frac{2}{[1 + \exp(\epsilon/2)]} \). The dots represent occupied sites and the fat lines are the cluster connections.

bosonic quantum spin systems [10, 11, 12], and the first cluster algorithm for lattice fermions was constructed in [13]. These algorithms can be implemented directly in the time continuum [7], i.e. the Suzuki-Trotter time discretization is not even necessary. In this study, we discretize the time direction.

We use the same algorithm that was used in [2]. Each configuration is decomposed into a set of clusters, which consist of connected lattice sites. A new configuration is generated by flipping the clusters. When a cluster is flipped, all lattice sites contained in that cluster change occupation number from \( n(x, t) \) to \( 1 - n(x, t) \), i.e. the occupied sites become empty and the empty ones occupied. To build the clusters, a probabilistic choice is made in each space-time interaction plaquette \([n(x, t), n(x + \hat{i}, t), n(x, t + 1), n(x + \hat{j}, t + 1)]\) as to which neighboring lattice sites are connected to one another. A cluster is a sequence of connected sites. In this algorithm, the clusters are closed loops. The probabilistic choices (called cluster break-ups) which build the clusters are designed to obey detailed balance and we only allow break-ups which generate legal plaquettes under cluster flips. The cluster rules are illustrated in Table 1. For plaquette configurations \([0, 0, 0, 0]\) and \([1, 1, 1, 1]\), i.e. entirely empty or entirely occupied, we always connect sites with their time-like neighbors. For configurations \([1, 0, 0, 1]\) and \([0, 1, 1, 0]\) where a fermion hops to a neighboring site, we always connect sites with their space-like neighbors. For configurations \([1, 0, 1, 0]\) and \([0, 1, 0, 1]\), i.e. a static fermion next to an empty site, we connect the sites with their time-like neighbors with probability \( p = \frac{2}{[1 + \exp(\epsilon/2)]} \) and with their space-like neighbors with probability \( 1 - p \). This algorithm was also
Figure 1: Two configurations of fermion occupation numbers in (1 + 1) dimensions. The dots represent occupied sites and the shaded plaquettes carry the interaction. With periodic spatial boundary conditions, the two fermions interchange positions in the second configuration, giving it $\text{Sign}[n] = -1$. Flipping the meron-cluster (represented by the fat line) changes one configuration into the other, changing the fermion sign.

Each cluster has two orientations, with lattice site occupancies $n(x, t)$ and $1 - n(x, t)$. When a cluster is flipped, the new configuration which is generated may have a different sign from the previous one, depending on whether or not the permutation of fermion world-lines is changed. A cluster whose flip changes $\text{Sign}[n]$ we call a meron, those which leave $\text{Sign}[n]$ unchanged we call non-merons. Flipping a meron changes the topology of the fermion world-lines. The term meron has been used before to denote half-instantons [15], such as in the 2-d $O(3)$ model at non-zero vacuum angle $\theta$ [16]. The number of merons in a configuration is always even, as flipping all clusters leaves the sign unchanged. An example of a meron-cluster is given in Figure 1. When the meron-cluster is flipped the first configuration with $\text{Sign}[n] = 1$ turns into the second configuration with $\text{Sign}[n] = -1$. For cluster algorithms more general than the one described here, it is not always possible to identify certain clusters as merons [17].

The meron concept alone gives us an exponential gain in statistics. Starting from a configuration containing $N_c$ clusters, we consider the ensemble of $2^{N_c}$ configurations where we allow all possible cluster orientations. If a configuration contains no merons, all configurations in the ensemble have $\text{Sign}[n] = 1$. However, if it contains merons, half the ensemble has $\text{Sign}[n] = 1$ and the other half $\text{Sign}[n] = -1$, which exactly cancel, giving a contribution 0. The improved estimator gives $\langle \text{Sign} \rangle = \langle \delta_{X,0} \rangle$, i.e. the probability that a configuration contains $N = 0$ merons, which is an expo-
ential improvement on standard algorithms, which measure a statistical average of $\pm 1$. As explained in [2], this solves half of the sign problem.

We also construct improved estimators for observables. The chiral susceptibility is

$$\chi = \frac{1}{\beta V} \langle (\bar{\Psi} \Psi)^2 \rangle_f = \frac{1}{\beta V} \frac{\langle (\bar{\Psi} \Psi)^2 \text{Sign} \rangle}{\langle \text{Sign} \rangle}.$$  

(3.1)

The total chiral condensate for a given configuration, $\bar{\Psi} \Psi[n] = \sum_C \bar{\Psi}_C$, is a sum of cluster contributions. Averaging $\chi$ over the ensemble of $2^{N_C}$ configurations gives

$$\chi = \frac{\langle \sum_C |\bar{\Psi}_C|^2 \delta_{N,0} + 2 |\bar{\Psi}_C| \|\bar{\Psi}_C\| \delta_{N,2} \rangle}{\beta V \langle \delta_{N,0} \rangle},$$  

(3.2)

This only gets contributions from configurations with $N = 0$ or $N = 2$ merons ($C_1$ and $C_2$ are the two merons). The vast majority of configurations contain many merons, but they make no contribution to observables. The zero- and two-meron sectors of configuration space are exponentially small, but they contain all of the contributions to $\chi$. Restricting ourselves to only explore this sub-space, we exponentially enhance both the numerator and denominator of eq.(3.2), leaving the ratio invariant. This solves the remaining half of the sign problem.

For the Binder cumulant $U$, we need to measure $\langle (\bar{\Psi} \Psi)^4 \rangle_f$ and hence

$$\langle \text{Sign} (\bar{\Psi} \Psi)^4 \rangle = \langle \text{Sign} \sum_{C_1, C_2, C_3, C_4} \bar{\Psi}_{C_1} \bar{\Psi}_{C_2} \bar{\Psi}_{C_3} \bar{\Psi}_{C_4} \rangle.$$  

(3.3)

A cluster’s condensate contribution $\bar{\Psi}_C$ changes sign when the cluster is flipped. When a meron-cluster is flipped, $\text{Sign}$ is changed. The non-zero terms in $\langle \text{Sign} (\bar{\Psi} \Psi)^4 \rangle$ do not change sign if any cluster in the configuration is flipped. These non-zero terms must contain odd powers of $\bar{\Psi}_C$ for all merons $C$ in the configuration and even powers of $\bar{\Psi}_{C'}$ for all non-merons $C'$. The average over the ensemble of $2^{N_C}$ configurations is

$$\langle \text{Sign} (\bar{\Psi} \Psi)^4 \rangle_{2^{N_C}} = \delta_{N,0} \left[ \sum_C |\bar{\Psi}_C|^4 + 6 \sum_{C, C'} |\bar{\Psi}_C|^2 |\bar{\Psi}_{C'}|^2 \right]$$

$$+ \delta_{N,2} \left[ 4 |\bar{\Psi}_{C_1}|^3 |\bar{\Psi}_{C_2}| + 4 |\bar{\Psi}_{C_2}|^3 |\bar{\Psi}_{C_1}| + 12 \sum_C |\bar{\Psi}_C|^2 |\bar{\Psi}_{C_1}| |\bar{\Psi}_{C_2}| \right]$$

$$+ \delta_{N,4} \left[ 24 |\bar{\Psi}_{C_1}| |\bar{\Psi}_{C_2}| |\bar{\Psi}_{C_3}| |\bar{\Psi}_{C_4}| \right],$$  

(3.4)

where $N$ is the number of merons in the configurations, $C_1, C_2, C_3$ and $C_4$ are the merons and all sums in eq.(3.4) are over non-meron clusters. This average only gets contributions from the zero-, two- and four-meron sectors and so we need only explore this sub-space. We average this quantity over the complete bosonic ensemble to measure $\langle \text{Sign} (\bar{\Psi} \Psi)^4 \rangle$ and hence $U$.  

9
Consider the case of measuring $\chi$. We expect that $p(0)/p(2) \propto (|C|/V\beta)^2$, where $p(0)$ and $p(2)$ are the probabilities that a configuration has zero or two merons and $|C|$ is the average cluster size. In large volumes, the majority of configurations has two merons, contributing 0 to $\langle \text{Sign} \rangle$. For even greater accuracy, we reweight the meron-sectors with trial probabilities $p_t(0)$ and $p_t(2)$, so that they appear with roughly equal frequency. This gives

$$\chi = \frac{\langle \sum_C |\bar{\Psi}_C|^2 \delta_{N,0} \ p_t(0) + 2|\bar{\Psi}_C_1||\bar{\Psi}_C_2|\delta_{N,2} \ p_t(2) \rangle}{\beta V \langle \delta_{N,0} \ p_t(0) \rangle}. \quad (3.5)$$

The reweighting probabilities can be adjusted to minimize the statistical error. This technique was previously used in \[16\]. To measure the Binder cumulant $U$, we use reweighting probabilities $p_t(0), p_t(2)$ and $p_t(4)$.

## 4 Numerical Results

We have performed simulations of the staggered fermion model on lattices with antiperiodic spatial boundary conditions from $L = 4$ up to $L = 30$ at inverse temperatures in the range $\beta \in [1.0, 3.0]$, which includes the critical temperature where the chiral symmetry is spontaneously broken. We have made separate runs with either a fixed number of time slices (typically $M = 10$, i.e. 40 time slices) or with fixed lattice spacing in the time direction ($\epsilon = 0.1$). In each simulation, we have made at least 1000 thermalization sweeps followed by 10000 measurements, with these numbers increased by a factor of 10 for $L \leq 10$. In one sweep of the lattice, a new cluster connection is proposed on each interaction plaquette and each cluster is flipped with probability $1/2$. To find the optimal reweighting probabilities $p_t(N)$ that minimize the statistical error, we first make a sample run without reweighting, only exploring the relevant meron-sectors. The observed relative weights are then used in production runs, where the sectors appear with equal probability. The major part of the sign problem is removed by the improved estimators, but reweighting is necessary for accurate measurements in large volumes.

A sample of the data measured is given in Table 2. The Table contains $\langle \text{Sign} \rangle$ and the susceptibility $\chi$ measured over all meron-sectors, and the reweighted $\langle \text{Sign} \rangle_r$ and $\chi_r$ measured over the zero- and two-meron sectors only with the reweighting factor $p_t(0)/p_t(2)$. All of these data are produced with 1000 thermalization sweeps and 10000 measurements. As all of the contributions to $\chi$ come from the zero- and two-meron sectors, $\chi$ and $\chi_r$ should be identical. Note that $\langle \text{Sign} \rangle_r$, the fraction of zero-meron configurations generated by sampling the zero- and two-meron sectors only, is typically a lot bigger than $\langle \text{Sign} \rangle$, the fraction of zero-meron configurations generated over all meron sectors. In small space-time volumes, $\chi$ can be accurately measured even when sampling all meron sectors. However, in large space-time volumes, $\langle \text{Sign} \rangle$ is too small to be measured and we can only determine
Table 2: Numerical results for the non-reweighted $\langle \text{Sign} \rangle$ and susceptibility $\chi$ measured over all meron sectors, and the reweighted $\langle \text{Sign} \rangle_r$ and $\chi_r$ measured over the zero- and two-meron sectors only with a reweighting factor $p_t(0)/p_t(2)$. For the larger volumes, $\langle \text{Sign} \rangle$ and $\chi$ cannot be measured.

| $L$ | $\beta$ | $\langle \text{Sign} \rangle$ | $\chi$ | $p_t(0)/p_t(2)$ | $\langle \text{Sign} \rangle_r$ | $\chi_r$ |
|-----|-----|------------------|-----|-----------------|-----------------|-----|
| 8   | 1.0 | 0.804(5)        |         | 0.5/0.5        | 0.820(7)        | 0.826(6) |
| 8   | 1.5 | 0.465(9)        | 2.84(3) | 0.5/0.5        | 0.52(1)         | 2.84(4) |
| 8   | 2.0 | 0.214(6)        | 9.2(2)  | 0.3/0.7        | 0.474(9)        | 9.0(1)  |
| 8   | 2.4 | 0.140(4)        | 16.6(3) | 0.2/0.8        | 0.501(9)        | 16.4(3) |
| 10  | 2.4 | 0.057(3)        | 24.8(6) | 0.2/0.8        | 0.369(8)        | 24.2(5) |
| 12  | 2.4 | 0.0203(8)       | 33(1)   | 0.1/0.9        | 0.443(7)        | 34.0(7) |
| 14  | 2.4 | 0.0052(6)       | 41(4)   | 0.1/0.9        | 0.338(8)        | 44(1)   |
| 16  | 2.4 | 0.0005(2)       | 80(40)  | 0.075/0.925    | 0.314(4)        | 57(1)   |
| 20  | 2.4 | —               | —       | 0.03/0.97      | 0.355(9)        | 82(3)   |
| 24  | 2.4 | —               | —       | 0.01/0.99      | 0.46(1)         | 120(5)  |
| 28  | 2.4 | —               | —       | 0.01/0.99      | 0.329(9)        | 156(8)  |

Figure 2: The meron number probability distribution for various spatial sizes $L = 8, 12, 20$ and $28$ at $\beta = 2.4$. 

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the susceptibility by restricting ourselves to the zero- and two-meron sectors. The staggered fermion model suffers from a very severe sign problem which is solved by the Meron-Cluster algorithm.

Figure 2 shows the meron number probability distribution in an algorithm that samples all meron sectors without reweighting. For small volumes the zero-meron sector and hence $\langle \text{Sign} \rangle$ are relatively large, while multi-meron configurations are rare. On the other hand, in larger volumes the vast majority of configurations has a large number of merons and hence $\langle \text{Sign} \rangle$ is exponentially small. For example, an extrapolation from smaller volumes gives a rough estimate for the non-reweighted $\langle \text{Sign} \rangle \approx 10^{-9}$ on the $L = 28$ lattice at $\beta = 2.4$, while the reweighted $\langle \text{Sign} \rangle_r = 0.329(9)$. Even if the configurations are entirely uncorrelated, to achieve a similar accuracy without the meron-cluster algorithm one would have to increase the statistics by a factor $10^{18}$, which is obviously impossible. In fact, at present there is no other method that can be used to simulate this model.

Figure 3 shows the chiral susceptibility $\chi$ as a function of $\beta$ for various spatial sizes $L$. At high temperatures (small $\beta$) $\chi$ is almost independent of the volume, indicating that chiral symmetry is intact. On the other hand, at low temperatures (large $\beta$) $\chi$ increases with the volume, which implies that chiral symmetry is spontaneously broken. To study the critical behavior in detail, we have performed a finite-size scaling analysis for $\chi$ focusing on the range $\beta \in [2.2, 2.6]$ around the
Figure 4: The chiral susceptibility plotted against $L$ for various values of $\beta$ computed with $\epsilon = 0.1$. The fit is to the finite-size scaling formula (4.1) with $a(x)$ expanded to first order and $b(y)$ expanded to third order. The exponents are set to the 2-d Ising model values. All curves are obtained from one fit. The $\chi^2$ per degree of freedom is 0.84 indicating a good agreement of our data with the finite-size scaling ansatz and 2-d Ising model critical exponents.

Critical point. Since a $\mathbb{Z}(2)$ chiral symmetry is spontaneously broken at finite temperature in this $(2+1)$-d model, one expects to find the critical behavior of the 2-d Ising model. The corresponding finite-size scaling formula valid close to $\beta_c$ is

$$\chi(L, \beta) = a(x) + b(y)L^{\gamma/\nu},$$

$$a(x) = a_0 + a_1 x + a_2 x^2 + ..., \ x = \beta - \beta_c,$$

$$b(y) = b_0 + b_1 y + b_2 y^2 + ..., \ y = (\beta - \beta_c)L^{1/\nu}. \ (4.1)$$

For the 2-d Ising model the critical exponents are given by $\nu = 1.0$ and $\gamma/\nu = 1.75$. Assuming these values for the exponents, we obtain $\beta_c = 2.43(1)$ for fixed $\epsilon = 0.1$ from the finite-size scaling fit, with a chi squared per degree of freedom of 0.84. The fit of the data is plotted in Figure 4. The value of $\beta_c$ is slightly dependent on $\epsilon$.

In the finite-size scaling equation (4.1), for large enough $L$ one can neglect the term $a(x)$. Then $\chi/L^{\gamma/\nu}$ is a function of $y = (\beta - \beta_c)L^{1/\nu}$ alone, i.e. the susceptibility
data in various volumes at various $\beta$ can be described by one universal function. We have varied the value $\beta_c$ to find if all the data can be collapsed onto one universal curve. In Figure 5, we plot the universal curve obtained by taking $\beta_c = 2.43$. The excellent agreement over a large range of spatial volumes $L$ and inverse temperatures $\beta$ is an indication of the quality of the finite-size scaling fit.

We also measure $U_L$, the Binder cumulant in volumes of extent $L$. In Figure 6, we plot the expected behavior of $U_L$ as $L$ increases for different temperatures. For $T > T_c$, the chiral symmetry is intact and $U_L$ flows into the $T = \infty$ fixed point $U = 0$. For $T < T_c$, the chiral symmetry is spontaneously broken and $U_L$ flows into the $T = 0$ fixed point $U = 2/3$. If the universality class has a non-trivial fixed point $U = U_*$, then $U_L$ flows into this value at $T = T_c$. By measuring $U_L$ in various volumes at many different temperatures, we determine this flow numerically. We have measured the Binder cumulant values in volumes up to $L = 30$ and we plot some of these values as a function of $1/L$ in Figure 7. These measurements are made with the number of time slices fixed at 40. Each curve in the figure represents some fixed temperature. In Figure 7, for small $\beta$ (i.e. high temperatures), $U_L$ clearly flows into the infinite temperature fixed point $U = 0$, while for $\beta$ large (low temperatures),
Figure 6: The expected flow of $U_L$ as a function of $1/L$. On each curve the temperature is constant.

Figure 7: Measured values of $U_L$ plotted versus $1/L$ for various $\beta$ in volumes with 40 time slices. Near $\beta = 2.35$, the values appear to flow into the non-trivial fixed point $U_\ast = 0.60(1)$. 
$U_L$ flows into the zero temperature fixed point $U = 2/3$. For $\beta$ close to $\beta_c$, we have to go to larger volumes to see this behavior. Near $\beta = 2.35$, the cumulant values appear to flow into a non-trivial fixed point $U_*$. Examining this region closely, we estimate the critical inverse temperature as $\beta_c = 2.36(2)$ and the fixed point value $U_* = 0.60(1)$. The finite-size scaling fit of $\chi$ measured at this $\epsilon \approx 0.24$ gives the same value of $\beta_c$. Note that this deviates slightly from the critical temperature measured at $\epsilon = 0.1$. The universal fixed point value for the 2-d Ising model is estimated as $U_* \sim 0.58$ [19]. This is further evidence that the chiral phase transition belongs to the 2-d Ising universality class.

5 Conclusions

The Meron-Cluster algorithm has recently been developed to allow numerical simulations in models which suffer from a very severe sign problem. In this paper, we have applied this technique to investigate a model of staggered fermions. Unlike standard methods, which integrate out the fermions, resulting in a non-local bosonic action, we use a Fock space of occupation number to describe the fermions. We have a local bosonic action, with an additional non-local sign factor which contains the Fermi statistics. Due to the Pauli exclusion principle, configurations which have an odd permutation of fermion world lines have a negative sign. This sign leads to very large cancellations in observables and usually makes it impossible to make accurate measurements in numerical simulations. The Meron-Cluster algorithm decomposes every configuration into closed loops of connected sites, each loop being a cluster. Loops which change the fermion sign when flipped are identified as meron-clusters. A meron-cluster identifies a pair of configurations with equal weight and opposite sign. This results in an exact cancellation of two contributions $\pm 1$ to the path integral, such that only configurations without merons contribute to the partition function. Observables only receive contributions from configurations which contain very few or no merons, whereas the vast majority of configurations contain many merons. By only exploring the sectors of configuration space with the relevant numbers of merons, one makes an exponential gain in statistics. Combined with efficient re-weighting of the remaining meron sectors, this completely solves the sign problem. Cluster algorithms are extremely efficient at exploring configuration spaces and generating uncorrelated configurations and generally do not suffer from critical slowing down. Even in models without a sign problem, the Meron-Cluster algorithm is more efficient than standard fermion simulation methods.

In this paper, we examined a model of $N = 1$ flavor of staggered fermions in $(2 + 1)$-dimensions, which has a $\mathbb{Z}(2)$ chiral symmetry. The model has a very severe sign problem and cannot be solved by standard fermion simulation algorithms. Using a Meron-Cluster algorithm, we were able to make high-precision measurements of the chiral susceptibility and Binder cumulant even in very large volumes and
low temperatures. In order to perform an accurate and reliable finite-size scaling analysis, it was necessary to go to volumes so large, where the sign problem is so severe, that a standard algorithm would require statistics on the order of $10^{18}$ to attain a similar accuracy. We were able to verify that the model undergoes a finite-temperature chiral phase transition, which belongs to the universality class of the $2-d$ Ising model. This is the behavior expected from dimensional reduction and universality. The same universal behavior was observed in the $N = 4$ flavor case \[5\]. However, the standard fermion algorithm that was used in that study does not work for $N < 4$ due to the fermion sign problem.

It is quite natural to use cluster algorithms in models of discrete variables. A future possible application of the Meron-Cluster algorithm is in exploring quantum link models \[20\] which are used in the D-theory formulation of QCD \[21, 22, 23\]. In D-theory, a model of discrete quantum variables undergoes dimensional reduction, resulting in an effective theory of continuous classical variables. In quantum link QCD the quarks arise as domain wall fermions. The application of meron-cluster algorithms to domain wall fermions is in progress. Also there are many applications to sign problems in condensed matter physics. Investigations of antiferromagnets in a magnetic field and of systems in the Hubbard model family are given in Ref.\[3\].

At present, the Meron-Cluster algorithm is the only method that allows us to solve the fermion sign problem. A severe sign problem arises in lattice QCD calculations at non-zero baryon number due to a complex action. It is therefore natural to ask if our algorithm can be applied to this case. At non-zero chemical potential the 2-d $O(3)$ model, which is a toy model for QCD, also suffers from a sign problem due to a complex action. When applied to the D-theory formulation of this model, the Meron-Cluster algorithm solves the sign problem completely \[3\]. It is an open question if such progress can be made in investigations of QCD.

Acknowledgements

We would like to thank Shailesh Chandrasekharan and Uwe-Jens Wiese for helpful discussions.

References

[1] S. Chandrasekharan and U.-J. Wiese, Phys. Rev. Lett. 83 (1999) 3116.
[2] S. Chandrasekharan, J. Cox, K. Holland and U.-J. Wiese, \texttt{hep-lat/9906021}.
[3] J. Cox, C. Gattringer, K. Holland, B. Scarlet, U.-J. Wiese, hep-lat/9909119; S. Chandrasekharan, B. Scarlet and U.-J. Wiese, cond-mat/9909451; S. Chandrasekharan, hep-lat/9909007 and hep-lat/0001003.

[4] J. B. Kogut, M. A. Stephanov and C. G. Strouthos, Phys. Rev. D58 (1998) 096001.

[5] J. B. Kogut and C. G. Strouthos, hep-lat/9904008

[6] L. Susskind, Phys. Rev. D16 (1977) 3031.

[7] B. B. Beard and U.-J. Wiese, Phys. Rev. Lett. 77 (1996) 5130.

[8] P. Jordan and E. Wigner, Z. Phys. 47 (1928) 631.

[9] N. D. Mermin and H. Wagner, Phys. Rev. Lett. 17 (1966) 1133; S. Coleman, Commun. Math. Phys. 31 (1973) 259.

[10] U.-J. Wiese and H.-P. Ying, Phys. Lett. A168 (1992) 143.

[11] H. G. Evertz, G. Lana and M. Marcu, Phys. Rev. Lett. 70 (1993) 875.

[12] H. G. Evertz, The loop algorithm, in Numerical Methods for Lattice Quantum Many-Body Problems, ed. D. J. Scalapino, Addison-Wesley Longman, Frontiers in Physics.

[13] U.-J. Wiese, Phys. Lett. B311 (1993) 235.

[14] U.-J. Wiese and H.-P. Ying, Z. Phys. B93 (1994) 147.

[15] C. G. Callan, R. Dashen and D. J. Gross, Phys. Lett. B66 (1977) 375.

[16] W. Bietenholz, A. Pochinsky and U.-J. Wiese, Phys. Rev. Lett. 75 (1995) 4524.

[17] S. Chandrasekharan, in preparation.

[18] H. W. J. Blöte, E. Luitjen and J. R. Heringa, J. Phys. A28 (1995) 6289.

[19] K. Binder, Phys. Rev. Lett. 47 (1981) 693.

[20] S. Chandrasekharan and U.-J. Wiese, Nucl. Phys. B492 (1997) 455.

[21] R. C. Brower, S. Chandrasekharan and U.-J. Wiese, Phys. Rev. D60 (1999) 094502.

[22] B. B. Beard, R. C. Brower, S. Chandrasekharan, D. Chen, A. Tsapalis and U.-J. Wiese, Nucl. Phys. B (Proc. Suppl.) 63 (1998) 775.

[23] U.-J. Wiese, Nucl. Phys. B (Proc. Suppl.) 73 (1999) 146.