Fermion-loop simulation of the lattice Gross-Neveu model

Christof Gattringer,[1] Verena Hermann,[1,2] and Markus Limmer[1]

[1]*Institut für Physik, FB Theoretische Physik, Universität Graz 8010 Graz, Austria*
[2]*Department of Earth and Environmental Sciences, Geophysics, Munich University 80333 Munich, Germany*

We present a numerical simulation of the Gross-Neveu model on the lattice using a new representation in terms of fermion loops. In the loop representation all signs due to Pauli statistics are eliminated completely and the partition function is a sum over closed loops with only positive weights. In the loop representation a different type of boundary condition appears: sectors of constant winding number. We demonstrate that the new formulation allows one to simulate volumes which are 2 orders of magnitude larger than those accessible with standard methods.

I. INTRODUCTION

Numerical simulations with fermions are notoriously difficult. The reason is that the minus signs due to Pauli statistics give rise to cancellation effects. In quantum field theories the fermions are usually integrated out and the fermion determinant appears as a weight factor. Even in cases where the fermion determinant is real and positive its numerical treatment is very costly, since it essentially couples all degrees of freedom with each other.

Finding alternative strategies for dealing with fermions would considerably improve the quality of numerical simulations. Such strategies could either be new algorithms (see, e.g., [1] for a prominent example) or a reformulation of the problem. Here we discuss the latter: In [2] an alternative representation was given for a two-dimensional fermionic quantum field theory, the Gross-Neveu model. The partition function was rewritten as a sum over closed loops where each contribution has a real positive weight. This allows for a new approach to simulate the model which avoids dealing with the fermion determinant.

This paper presents the first test of the loop approach for the Gross-Neveu model in a numerical simulation, and we explore the prospects and limitations of using loop-type representations in a numerical simulation of a fermionic system. Our results demonstrate that the method is promising and it is worthwhile to pursue it in higher dimensions. In higher dimensions loop representations of quantum field theories are known, but so far have exclusively been used in the strong coupling limit [3]. Our study here, although 2-dimensional, is performed at arbitrary coupling. We are currently exploring the generalization to higher dimensions and believe that for certain four-fermi interactions, representations similar to the one used here can be found and successfully applied in numerical simulations.

For gauge theories the situation is more complicated. Since gauge fields are oriented one has to use oriented loops dressed with the gauge links and complex phases appear. This was seen in the Schwinger model, where a loop representation exists [4], but a numerical simulation suffers from the fermion sign problem. Upon going to the strong coupling limit, the sign problem disappears [5] and a numerical simulation with loops again unleashes its power [6]. Four-fermi interactions may be generated with a Hubbard-Stratonovich transformation using scalar fields. These do not introduce complex phases and a loop representation without signs is possible.

II. THE LOOP REPRESENTATION

We begin with discussing the Gross-Neveu model [7] and its loop representation. In the continuum the action of the Gross-Neveu model is given by $S = S_F + S_S$ with

$$S_F = \int d^2x \bar{\psi}(x)[\gamma_\mu \partial_\mu + \varphi(x) + m]\psi(x),$$
$$S_S = \frac{1}{2g} \int d^2x \varphi(x)^2. \tag{1}$$

Here ψ and $\bar{\psi}$ are Grassmann valued vectors of N flavors of 2-spinors and we use vector/matrix notation for both, spinor and flavor indices. The Euclidean partition function is defined by integrating over all fields,

$$Z = \int \prod_x d\varphi(x) d\bar{\psi}(x)\psi(x) \exp(-S[\varphi, \bar{\psi}, \psi]). \tag{2}$$

Upon integrating out the scalar fields φ, the model turns into a purely fermionic theory with a 4 Fermi interaction given by $-g/2 \int d^2x(\bar{\psi}(x)\psi(x))^2$. The Gross-Neveu model is well understood analytically (see e.g. [8]) and has been analyzed on the lattice in various settings [9].

As it stands, the path integral (2) is only formally defined and a cutoff needs to be introduced. Here we use lattice regularization, which replaces the Euclidean space time $\mathbb{R}^2$ by a finite regular lattice Λ. The path integral (2) is well defined when the measure is understood as the product over individual measures over the fields living on the lattice points. The action is discretized using the Wilson formulation such that it reads

$$S_F = \sum_{x \in \Lambda} \bar{\psi}(x) \left(- \sum_{\mu = \pm 1}^{\pm 2} \frac{1 \mp \gamma_\mu}{2} \psi(x \pm \hat{\mu}) + \varphi(x)\psi(x) \right.$$

$$\left. + [2 + m]\psi(x) \right),$$

$$S_S = \frac{1}{2g} \sum_{x \in \Lambda} \varphi(x)^2. \tag{3}$$

For the scalar field φ we use periodic boundary conditions for both directions, the fermions are periodic in the spatial direction and antiperiodic in time.

Using hopping expansion techniques, the N-flavor lattice Gross-Neveu model (3) can be mapped into a model of $2N$ sets of loops [2]. For convenience we will often refer to the loops in different sets as blue, red, etc. loops. Within each set the loops are nonoriented, closed, and self-avoiding. However, when loops belong to different sets, e.g., a red and a blue loop, they may touch or cross each other. The partition function of the lattice Gross-Neveu model is then a sum over all possible configurations of the loops in the $2N$ sets. Each configuration has a positive weight computed from the loops.

Although [2] gives the partition function for arbitrary N, we here only quote the one-flavor expression which we use in our simulation. We remark that for $N = 1$ the 4-fermi interaction is equivalent to the interaction of the Thirring model. For $N = 1$ the model is invariant under continuous chiral rotations, while for $N > 1$ only a discrete symmetry remains. Thus the physics for $N = 1$ is different from the $N > 1$ case, where the model is asymptotically free.

For the loop representation at $N = 1$ we need two sets of self-avoiding loops, red and blue, denoted by r and b. The one-flavor partition function in the loop representation reads (up to an overall normalization factor)

$$Z = \sum_{r,b} (1/\sqrt{2})^{c(r,b)} f_1^{n_1(r,b)} f_2^{n_2(r,b)}. \tag{4}$$

In this formula $c(r, b)$ is the total number of corners for both red and blue loops. Thus every corner contributes a factor of $1/\sqrt{2}$ to the weight of a configuration. $n_1(r, b)$ is the number of lattice sites which are singly occupied by either r or b and $n_2(r, b)$ is the number of doubly occupied sites. We remark that, since the loops in the two sets are self-avoiding, double occupation can appear only when a red and a blue loop cross or run alongside each other. The weight factors f_1 and f_2 are related to the mass m and the coupling g through

$$f_1 = (2 + m)[(2 + m)^2 + g]^{-1},$$
$$f_2 = [(2 + m)^2 + g]^{-1}. \tag{5}$$

We stress that the mapping (4) and (5) is exact in the thermodynamic limit. For finite volume different types of boundary conditions in the two representations lead to finite size effects: In the loop representation we need to have closed loops and in a finite volume the loops can wind around the periodic boundary. The loop configurations fall into three equivalence classes, C^{ee}, C^{eo}, C^{oo}, depending on the numbers of red and blue nontrivially winding loops (see also [6]): C^{ee} (even-even): The total number of windings for both, red and blue loops is even for both directions. C^{eo} (even-odd): One of the colors has an odd number of windings for one of the directions. C^{oo} (odd-odd): Both colors have an odd number of windings in one of the directions. These equivalence classes cannot be linked in a simple way to the boundary conditions in the standard representation which we discussed above. However, below we will demonstrate that the boundary effects vanish as $1/\sqrt{V}$, with V denoting the volume.

III. NUMERICAL SIMULATION

The numerical simulation of the Gross-Neveu model now is performed directly in the loop representation (4) using a local Metropolis update (see e.g. [10]). We update the red and the blue loops alternately, by performing a full sweep through the lattice for one of the colors and treating the other one as a background field. A sweep consists of visiting all plaquettes of the lattice. For each plaquette we generate a trial configuration by inverting the occupation of the color we want to update for all the links in the plaquette. This guarantees that all loops remain closed. Furthermore new loops may be generated when all links of the plaquette are empty. When the trial configuration violates the self-avoiding condition it is rejected immediately and the algorithm tries the next plaquette. Otherwise the trial configuration is accepted with the Metropolis probability $p = (1/\sqrt{2})^{\Delta c} f_1^{\Delta n_1} f_2^{\Delta n_2}$, where Δc is the change in the number of corners and $\Delta n_1, \Delta n_2$ are the changes in the occupation numbers. The initial configuration can either be the empty lattice (for C^{ee}) or has one or two winding loops (C^{eo} and C^{oo}).

The observables we discuss here are all first and second derivatives of the free energy $F = -\ln Z$ and can be written as moments of the occupation numbers. In particular, for the chiral condensate and its susceptibility, which in the standard language are given by

$$\chi = \frac{1}{V} \sum_{x \in \Lambda} \langle \bar{\psi}(x)\psi(x) \rangle = -\frac{1}{V} \frac{\partial \ln Z}{\partial m}, \qquad C_\chi = \frac{\partial \chi}{\partial m}, \tag{6}$$

we quote the corresponding expressions in terms of occupation numbers and their fluctuations,

$$\chi = -\frac{1}{Vf_1}(f_2 \langle n_1 \rangle + 2f_1^2 \langle n_0 \rangle),$$

$$C_\chi = -\frac{1}{Vf_1^2}([4f_1^4 - 2f_1^2 f_2]\langle (n_0 - \langle n_0 \rangle)^2 \rangle$$
$$+ [f_2^2 - 2f_1^2 f_2]\langle (n_1 - \langle n_1 \rangle)^2 \rangle + 2f_1^2 f_2 \langle (n_0 + n_1$$
$$- \langle n_0 + n_1 \rangle)^2 \rangle - [4f_1^4 - 2f_1^2 f_2]\langle n_0 \rangle - f_2^2 \langle n_1 \rangle). \tag{7}$$

Here we have introduced n_0, the total number of empty sites, i.e., sites visited by neither a red nor a blue loop.

Equivalent formulas can be derived for the internal energy, the heat capacity as well as for derivatives of the free energy with respect to the coupling g. n-point functions may be treated as usual by introducing source fields and differentiating with respect to them. This gives expressions involving correlators of *local* occupation numbers. Finally, the generalization of the above formulas to an arbitrary number of flavors is straightforward.

IV. RESULTS

In this section we present some selected results which serve to illustrate the advantages of the loop approach, but also allow us to assess its limitations. In order to compare with traditional methods, we performed a reference simulation of the Gross-Neveu model using standard methods. The fermions were integrated out giving rise to the fermion determinant in a background configuration of the scalar field φ. These background configurations were computed according to the Gaussian distribution of S_S, and the determinant was used as a factor for reweighting. This is possible, since the eigenvalues of the Dirac matrix come in complex conjugate pairs, and the scalar field does not have topological modes which could give rise to zero eigenvalues. Thus the fermion determinant is always strictly positive.

We stress that the reweighting in the standard formulation works only in two dimensions due to the numerical cost of evaluating the determinant. However, for our problem where the scalar fields are independent Gaussians at each site, reweighting has the big advantage, that autocorrelation is avoided. Alternative strategies such as Hybrid Monte Carlo cannot make use of that advantage.

Another important conceptual point has to be addressed: For the free case, $g = 0$, the standard representation allows for an exact solution with the help of Fourier transformation (where we use antiperiodic boundary conditions in time direction and periodic ones in the space direction). In the loop formulation, however, the case $g = 0$ is not special at all. Thus $g = 0$ is the optimal point for testing the power of the loop approach to the limits because we have exact results on almost arbitrary large volumes, which we use to compare with the data of the loop simulation. Since the weight factors f_1 and f_2 of Eq. (5) are smooth functions of g and m it is reasonable to transfer the experience obtained with the loop approach at $g = 0$ to nearby values of g.

Thus we begin our assessment of the loop approach at $g = 0$. In Figs. 1 and 2 we compare the loop results in the C^{ee} sector (symbols) with those from Fourier transformation (curves). We use two volumes for the comparison, a relatively small lattice of size 32×32 and a considerably larger one, 512×512. For the simulation in the loop approach at each value of m we typically performed
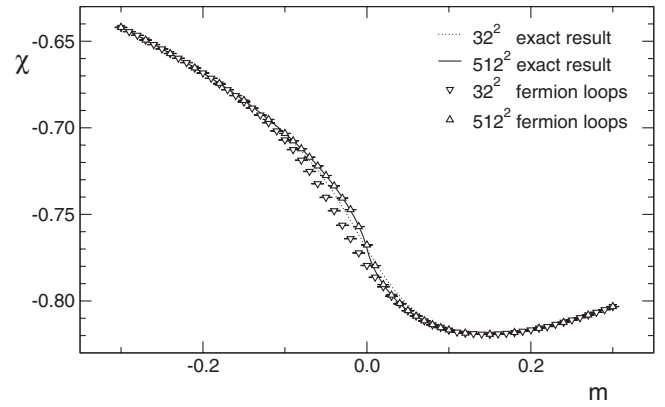

FIG. 1. The chiral condensate χ for $g = 0$ as a function of m for 2 different lattice sizes. We compare the simulation in the loop representation (symbols with error bars) to the exact result from Fourier transformation (curves).

10 000 sweeps of our local update for both colors for equilibration and used 50 000 measurements of the observables separated by 10 pairs of sweeps. The observables were calculated using the occupation number representation (7) and the statistical error was computed with the jackknife method.

Figure 1 shows that already on the small lattice the data points are very close to the exact result. The largest discrepancy is seen near $m = 0$, the chiral point where the fermions become massless. For the larger lattice the data points fall exactly on top of the analytic result. The situation is similar for the susceptibility in Fig. 2. For the small lattice we find a clear finite size effect, a shift of the susceptibility curve. On the larger lattice the agreement is almost perfect and only at the chiral point $m = 0$ we still see a slight discrepancy. We remark, that the decrease of the minimum of C_χ with increasing volume V does not signal a phase transition (at $N = 1$ there is no discrete symmetry that could be broken spontaneously). The minima decrease only logarithmically with V. For $g = 0$ it can be shown exactly that C_χ diverges logarithmically when
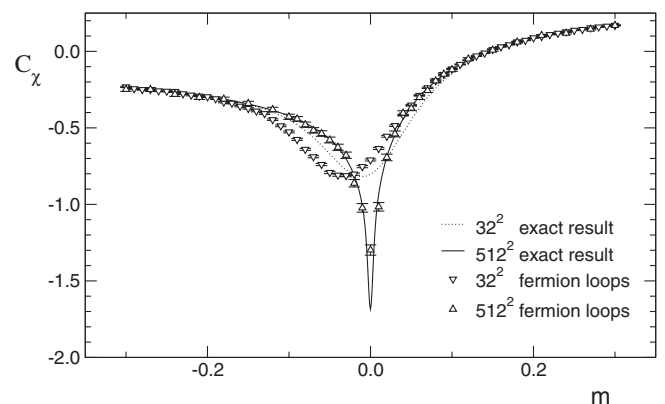

FIG. 2. Same as Fig. 1, now for the chiral susceptibility C_χ.
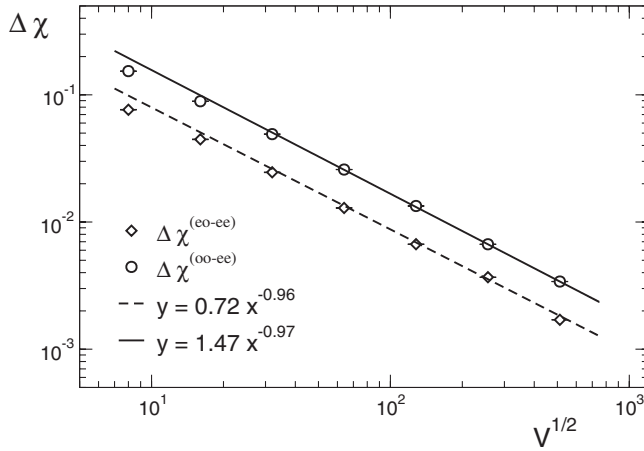
FIG. 3. Splitting of the results for the chiral condensate in the different equivalence classes as a function of the volume.

removing the IR cutoff. For $g > 0$ we could fit the minimum of C_χ as obtained from the simulation very reliably with $\ln V$. Also the comparison with the results from the standard approach shows that the largest discrepancy is found near the chiral point, which, however, vanishes quickly with increasing volume.

An important part of comparing the standard and the loop approach is to test how the different types of boundary effects scale with the volume and at what rate the perfect equivalence of the two representations is reached with increasing V. We assess this question directly in the loop approach: At a fixed point (m, g) in parameter space we compute the chiral condensate χ for the three different equivalence classes C^{ee}, C^{eo}, C^{oo} introduced above. This is repeated for several volumes V and in Fig. 3 we plot the discrepancy of the results as a function of $\sqrt{V}$. The data shown in the plot are for $g = 0.1$ and $m = 0.0$. In the plot $\Delta\chi^{(eo-ee)}$ denotes the discrepancy between the C^{eo} and C^{ee} results and $\Delta\chi^{(oo-ee)}$ is the splitting between C^{oo} and C^{ee}. Also a comparison of χ to the results from the standard approach with mixed boundary conditions shows a $1/\sqrt{V}$ behavior. The observed $1/\sqrt{V}$ behavior is what one expects for free massless Wilson fermions and our data indicate that this behavior persists at $g = 0.1$.

The splitting $\Delta\chi$ can be analyzed with the help of mean field theory. One finds that it should behave as $\Delta\chi \propto 1/\sqrt{V}$. We performed a fit of our data to the form $\Delta\chi \propto cV^\alpha$ and found values of α which are close to $-1/2$ for all analyzed values of (m, g) (see also Fig. 3). Thus mean field arguments as well as our numerical findings indicate that the finite volume effects scale as $1/\sqrt{V}$.

V. DISCUSSION

In this paper we have explored an alternative formulation for fermionic systems using the example of a 2-dimensional quantum field theory. The representation in terms of fermion loops allows one to simulate the system without having to use fermion determinants. An important aspect is that in the loop formulation used here we are not restricted to the case of strong coupling but can work at arbitrary g. In this exploratory study we simulate the model using a simple local update and compare the outcome to analytic results and the data from a simulation in the standard approach. Many observables can be expressed in terms of occupation numbers and their correlators. We show that finite size effects decrease like $1/\sqrt{V}$ and thus the thermodynamic limit, where the loop representation becomes exact, is approached rapidly.

An important issue is of course the assessment of the gain in numerical efficiency when using the loop algorithm. Already with the local algorithm used here a considerable increase of the accessible volumes was found. Using the same small computer cluster, the standard approach could be used on lattices with a maximum volume of 32×64, while in the loop formulation we were able to simulate systems up to 700×700, which is an increase of the volume by more than 2 orders of magnitude. This enormous improvement is a strong incentive to search for loop representations also in higher dimensional fermion systems and for four-fermi interactions no principal obstacles seem to appear.

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