Karl-Franzens Universität Graz

Institut für Physik, Fachbereich Theoretische Physik

Monte–Carlo simulation of the lattice Gross–Neveu model: Standard representation vs. fermion loops

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

[1] Karl–Franzens Universität, Graz [2] Ludwig–Maximilians Universität, Munich

Motivation

The numerical treatment of fermions is a long standing problem in lattice QCD. In the usual approach, the fermions are formally integrated out and the fermion determinant is evaluated. This fermion determinant is then taken into account as an additional weight factor in the Monte–Carlo simulation. Since the calculation of this determinant is plagued by the *fermion sign problem*, it is numerically very costly [1]. Thus, finding an alternative formulation of the problem would be enormously helpful. One possible alternative is the *fermion loop representation*. This approach is explored here for a lower dimensional model, namely the *Gross–Neveu model* [2].

Theoretical framework

We work with the 2d lattice version of the Gross–Neveu model for one flavor. The action of this model is given by

$$S = \sum_{\mathbf{n}\in\Lambda} \overline{\psi}(\mathbf{n}) \Big(\sum_{\mu=\pm 1}^{\pm 2} \frac{1 \pm \gamma_\mu}{2}\, \psi(\mathbf{n} \pm \hat{\mu}) \,+\, \big[2 + m + \phi(\mathbf{n})\big]\, \psi(\mathbf{n}) \Big) \,+\, \frac{1}{2g} \sum_{\mathbf{n}\in\Lambda} \phi(\mathbf{n})^2 \,,$$

where ϕ is a scalar background field and m and g are the bare mass and the coupling constant. The sums run over all lattice points $\mathbf{n}$ of the lattice Λ. The fermion fields $\overline{\psi}$, ψ are Grassmann valued 2–spinors.

The Euclidean partiton function is obtained by integrating $\exp(-S[\overline{\psi}, \psi, \phi])$ over all three types of fields. By integrating out only the scalar field ϕ, one gets a purely fermionic theory with the quartic interaction term

$$-\frac{g}{2} \sum_{\mathbf{n}} \Big[\, \overline{\psi}(\mathbf{n})\, \psi(\mathbf{n}) \,\Big]^2 \,.$$

On the lattice one can use hopping expansion techniques to map this model onto a model of 2 sets of loops [3]. These two sets will subsequently be referred to as "red" (r) and "blue" (b) loops. The loops of each single set are non–oriented, closed and self–avoiding. Loops of different colors, however, do not have to respect this self–avoidance. The partition function for the fermion loop representation is then a sum over all possible configurations of the loops in the two sets, more precisely

$$Z = \sum_{r,b} \left(\frac{1}{\sqrt{2}}\right)^{c(r,b)} f_1^{n_1(r,b)}\, f_2^{n_2(r,b)} \,.$$

Here, c is the total number of corners in both sets and n_1, n_2 are the number of singly or doubly occupied sites, respectively. The functions f_1 and f_2 are simple functions of the mass parameter m and the coupling constant g,

$$f_1 = \frac{2+m}{(2+m)^2+g} \,, \qquad f_2 = \frac{1}{(2+m)^2+g} \,.$$

Finally, we have a partition function which is a sum over terms with only real and positive weights! Thus, all problems due to signs, coming from the Pauli statistics, are gone. This mapping is exact in the thermodynamic limit. For finite lattice volumes the loop configurations can be divided into three different equivalence classes. The finite size effects therefrom vanish, however, like $1/\sqrt{V}$, for V being the lattice volume.

Numerical Simulation

The numerical simulation is done for both approaches, the standard representation and the fermion loop formalism. In the loop approach a local Metropolis update is used, in which red and blue loops are updated alternately. Thus, a full sweep through the lattice is performed for one color and meanwhile the other color serves as background field. As observables we use first and second order derivatives of the free energy $F = -\ln Z$. For the fermion loops these expressions can be written in terms of moments of occupation numbers. The conventional definition of the chiral condensate χ and susceptibility C_χ are

$$\chi \;=\; -\frac{1}{V}\frac{\partial \ln Z}{\partial m} \;=\; \frac{1}{V} \sum_{\mathbf{n}} \Big\langle \overline{\psi}(\mathbf{n})\, \psi(\mathbf{n}) \Big\rangle \,, \qquad C_\chi \;=\; \frac{\partial \chi}{\partial m} \,.$$

In the fermion loop approach we have

$$\begin{aligned} \chi &= -\frac{1}{V f_1} \Big[f_2 \langle n_1 \rangle \,+\, 2 f_1^2 \langle n_0 \rangle \Big] \,, \\ C_\chi &= -\frac{1}{V f_1^2} \Big[(4 f_1^4 - 2 f_1^2 f_2) \Big\langle (n_0 - \langle n_0 \rangle)^2 \Big\rangle \,+\, (f_2^2 - 2 f_1^2 f_2) \Big\langle (n_1 - \langle n_1 \rangle)^2 \Big\rangle \\ &\quad + 2 f_1^2 f_2 \Big\langle (n_0 + n_1 - \langle n_0 + n_1 \rangle)^2 \Big\rangle \,-\, (4 f_1^4 - 2 f_1^2 f_2) \langle n_0 \rangle - f_2^2 \, \langle n_1 \rangle \Big] \,. \end{aligned}$$

The number n_0 is the total number of empty lattice sites.

Results

Results from the loop approach are compared to those from a simulation using the standard representation. The results for that "benchmark simulation" are produced using the reweighting technique for the fermion determinant. In the free case $g = 0$ we make use of Fourier transformation and thus obtain exact results in the standard approach. In the loop formalism this case is not special at all. Thus, the point $g = 0$ is the optimal testing point, because exact results are available for almost arbitrarily large lattice volumes.

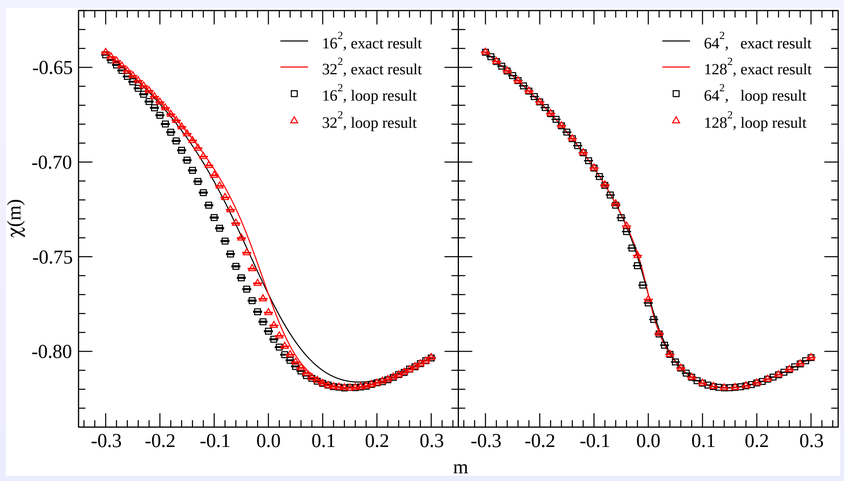

Fig. 1: *The chiral condensate χ for $g = 0$ as a function of m. On the l.h.s. we plot the lattice volumes 16^2 and 32^2, on the r.h.s. 64^2 and 128^2 can be found.*

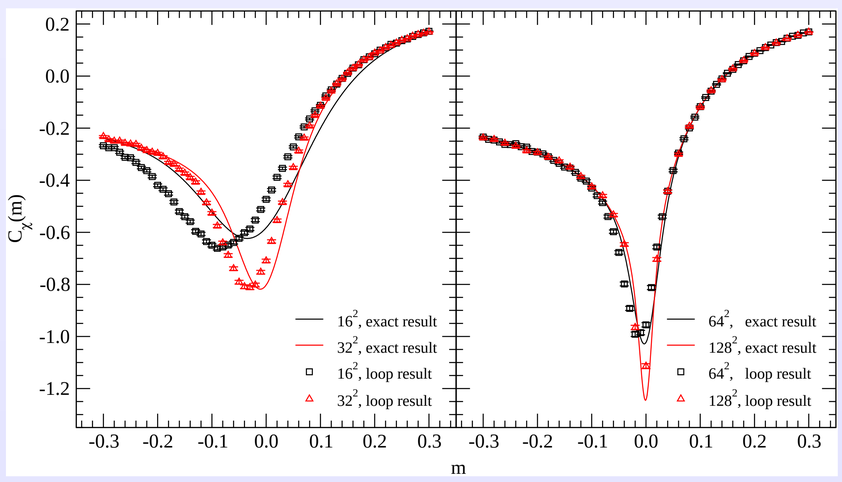

Fig. 2: *Same as Fig. 1, now for the chiral susceptibility C_χ.*

In Fig. 1 we show results for the chiral condensate χ for several lattice volumes. The different data sets agree very well for lattice sizes 32^2 and larger. The largest gap between the data is found near $m = 0$, the chiral point, where the fermions become massless. For bigger lattices the loop results fall exactly on top of the analytic results.

The situation for the chiral susceptibility is similar, see Fig. 2. There the discrepancy is getting acceptable from a lattice size of 64^2 on. The reason for this discrepancy in the two approaches are finite size effects from different types of boundary conditions for the loop approach (i.e., the above discussed equivalence classes). A much more detailed discussion of that analysis can be found in [4], a further development is [5].

Summary

We have explored an alternative formulation for fermionic systems using the example of the Gross–Neveu model. The representation in terms of fermion loops allowed us to simulate the system without having to evaluate the fermion determinant.

Here, we simulated the model using a simple local update and compared the outcome to analytic results from Fourier transformation. We saw 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. 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 two orders of magnitude! This enormous improvement is a strong incentive to search for loop representations also in higher dimensional fermionic systems.

References

[1] S. Chandrasekharan and U. J. Wiese, Phys. Rev. Lett. **83**, 3116 (1999).

[2] D. J. Gross and A. Neveu, Phys. Rev. **D10**, 3235, (1974).

[3] C. Gattringer, Nucl. Phys. **B543**, 533, (1999); Int. J. Mod. Phys. **A14**, 4853, (1999).

[4] C. Gattringer, V. Hermann, and M. Limmer, Phys. Rev. **D76**, 014503 (2007).

[5] U. Wolff, arXiv:0707.2872v1 [hep-lat]