Study of the complex fermion determinant in a $U(1)_L \otimes U(1)_R$ symmetric Yukawa model

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Abstract

Lattice theories that contain chiral multiplets of fermions can have complex fermion determinants. This is for example the case for the $U(1)_L \otimes U(1)_R$ symmetric Yukawa model with mirror fermions, if the number of generations of fermions and mirror fermions is odd. Whether a numerical simulation of such a model is possible depends on the magnitude of fluctuations of the complex phase factor of the fermion determinant. We investigate the fermion determinant of the $U(1)$ Yukawa model with mirror fermions for a physically relevant choice of parameters. The argument of the complex phase turns out to fluctuate only very little and is at most of the order of $2 \cdot 10^{-3}$.

1 Introduction

The problem of formulating theories with a chiral fermion content on a lattice has not yet been solved in a satisfactory way. As is well known lattice fermions are accompanied by unwanted doublers which one likes to remove at least in the continuum limit. Their appearance is related to the Nielsen-Ninomiya theorem [4], which requires that to every lattice fermion with a given set of quantum numbers a mirror fermion with the same quantum numbers but opposite parity exists. For a naive discretisation of the fermion action half of the doublers play the role of mirror fermions [4].

The Wilson term [3], which achieves the removal of doublers in vectorlike theories, spoils chiral invariance and cannot be used directly in chiral theories. For fermions interacting with scalar fields via Yukawa interactions a chiral invariant Wilson-Yukawa term has been proposed [4], but there is evidence that it does not fulfill its goal [6]. On the other hand it is possible to remove the doublers in chiral Yukawa models with the help of
a Wilson-like term but at the cost of introducing extra mirror fermions [3]. This yields the minimal possible proliferation of extra fermions. If one does not like to have the mirror fermions in the physical spectrum, even at a higher mass scale, the task is to find out whether the mirror fermions can be removed or decoupled in the continuum limit.

If gauge fields are neglected, chiral Yukawa models with mirror fermions are for a particular choice of parameters invariant under a Golterman-Petcher shift symmetry [7] with respect to the mirror fermion field [8]. As a result the mirror fermions decouple from the fermions and from the scalar field. It remains a truly chiral set of fermions interacting with the scalar field.

For a numerical simulation of such theories with the Hybrid Monte Carlo algorithm, however, the fermion fields have to be duplicated again. This is due to the following fact. The part of the action bilinear in the fermion fields can be written with the help of the “fermion matrix” $Q(\phi)_{xy}$ as

$$S_f = \sum_{x,y} \bar{\Psi}_x Q(\phi)_{xy} \Psi_y,$$

where

$$\Psi_x = \begin{pmatrix} \psi_x \\ \chi_x \end{pmatrix}$$

contains fermion fields $\psi$ and mirror fermion fields $\chi$, and $\phi$ is the complex scalar field. The matrix $Q$ is not necessary positive definite, while the hybrid Monte Carlo algorithm requires a positive definite fermion matrix. A duplication of fermion fields by introducing two generations $\Psi^{(1)}$ and $\Psi^{(2)}$ with opposite chirality amounts to replacing $Q$ by $Q^+Q$ and ensures the positive definiteness. This duplication is of a purely algorithmic origin and has nothing to do with the fermion doubling problem. Therefore it is desirable to find ways to simulate these models without additional duplication.

In particular, for a $U(1)_L \otimes U(1)_R$ symmetric model the determinant of $Q$ is in general complex, preventing a simulation of this model with standard Monte Carlo algorithms. Nevertheless a simulation without duplication would be possible depending on the fluctuations of the phase angle $\alpha$ of the fermion determinant. Two possible situations can be imagined:

1. the angle $\alpha$ fluctuates only very little about zero. Then a simulation with $|\det Q|$ appears feasible and the phase factor $\exp i\alpha$ can be put into the observables or neglected completely.

2. $\alpha$ fluctuates strongly and a simulation without taking the phase of $\det Q$ into account is not possible.

In order to find out which of these two possibilities holds we have investigated the fermion determinant in the $U(1)_L \otimes U(1)_R$ symmetric Yukawa model with mirror fermions.
2 Calculation of the fermion determinant

The U(1)$_L$ $\otimes$ U(1)$_R$ symmetric Yukawa model with mirror fermions has been considered in ref. [9] in detail and we refer to this article for the definition of the action and the parameters. The $8 \otimes 8$ matrix $Q$ is given in a $2 \otimes 2$ block notation by

$$Q(\phi)_{xy} = \delta_{xy} \begin{pmatrix}
G_\psi \phi_x^+ & 0 & 1 & 0 \\
0 & G_\psi \phi_x & 0 & 1 \\
1 & 0 & G_\chi \phi_x & 0 \\
0 & 1 & 0 & G_\chi \phi_x^+
\end{pmatrix}$$

$$- K \sum_\mu \delta_{x,y+\hat{\mu}} \begin{pmatrix}
0 & \Sigma_\mu & r & 0 \\
\bar{\Sigma}_\mu & 0 & 0 & r \\
r & 0 & 0 & \Sigma_\mu \\
0 & r & \bar{\Sigma}_\mu & 0
\end{pmatrix}. \quad (3)$$

Here $x$ and $y$ are lattice points, the sum $\sum_\mu$ runs over eight directions of the neighbours, and $\hat{\mu}$ is the unit vector in the direction of $\mu$. The Euclidean $\gamma$-matrices are expressed in a chiral basis as

$$\gamma_\mu = \begin{pmatrix}
0 & \Sigma_\mu \\
\Sigma_\mu & 0
\end{pmatrix}, \quad \gamma_5 = \begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix}. \quad (4)$$

For $\mu = 1, 2, 3$ we have $\Sigma_\mu = -\bar{\Sigma}_\mu = -i\sigma_\mu$ and $\Sigma_4 = \bar{\Sigma}_4 = 1$, where $\sigma_{1,2,3}$ denote the Pauli-matrices. For negative indices the definition is given by $\Sigma_\mu \equiv -\Sigma_{-\mu}$. The Yukawa couplings of the fermions and mirror fermions are $G_\psi$ and $G_\chi$, respectively. The term proportional to $Kr$ is a chiral invariant Wilson-term which serves to give the fermion doublers masses of the order of the cutoff. The Wilson parameter $r$ is set equal to 1 usually. Finally $K$ is the fermionic hopping parameter, whose critical value is 1/8 for vanishing Yukawa couplings.

The hybrid Monte Carlo algorithm requires the inversion of $Q$, which is done by conjugate gradient or minimal residue algorithm. A calculation of the determinant of $Q$ is more demanding. Straightforward application of standard determinant algorithms is not possible owing to the need of large storage. We proceeded in the following way. Let $L_i, \ i = 1, 2, 3, 4$ be the size of the lattice in the direction $i$. We consider even $L_i$ and set $L_4 = 2n$. $Q$ can be considered as a $2n \times 2n$ matrix consisting of block matrices belonging to time slices. Each block itself is a $M \times M$ matrix with $M = 8L_1L_2L_3$. In a first step the matrix is reordered by an even number of exchanges of rows and columns such that a
band structure is obtained:

\[
\begin{pmatrix}
  m_{T(1)} & b & a \\
  a & m_{T(2)} & 0 & b \\
  b & 0 & m_{T(3)} & 0 & a \\
  a & 0 & m_{T(4)} & 0 & b \\
  b & 0 & \cdots & & & \\
  \vdots & & & & & \\
  \pm b & m_{T(2n-1)} & a & \pm a & b & m_{T(2n)} \\
\end{pmatrix}.
\]

The blocks \(a\) and \(b\) are constant, whereas the \(m_j\) depend on the scalar field \(\phi\). The indicated signs near the lower right corner depend on the temporal boundary conditions. \(T(j)\) is a permutation of the time slices defined by

\[
T(1) = n, \quad T(2n) = 2n,
\]

\[
T(2j) = n - j, \quad T(2j + 1) = n + j \quad \text{for } j = 1, \ldots, n - 1.
\]

The matrix above is now dealt with by LU-block factorisation \([10]\). The resulting upper triangular matrix has blocks \(D_k\) on its diagonal, which can be determined recursively from the blocks \(m_j, a\) and \(b\). The complete determinant is given by

\[
\det Q = \prod_{k=1}^{2n} \det D_k.
\]

The “little” matrices \(D_k\) are not sparse. But for a \(4^3 \cdot L_4\) lattice they are small enough such that their determinants can be calculated by standard numerical routines. Similar techniques have been used by Toussaint as indicated in \([11]\).

The storage needed does not depend any longer on \(L_4\) and amounts to 6144(\(L_1L_2L_3\))^2 bytes using complex extended precision. In our case this is slightly more than 3 Megawords, which means a reduction by a factor of about 1/10 compared to a standard treatment. The CPU time is proportional to \(L_4\) instead of \(L_4^3\), which standard routines require. For \(L_4 = 8\) it takes 3 minutes to calculate one determinant on the Cray Y-MP with a high degree of vectorisation (300 MFlops).

Because the correctness and precision of the algorithm is crucial we have tested it in different ways:

1. For lattices smaller than \(4^4\) a comparison with the results obtained with the help of IMSL-library routines has been made.

2. For constant scalar fields \(\phi\) the determinant can be calculated exactly by Fourier transformation, and we compared with the resulting values.
3. The relation
\[
\frac{d}{d\lambda} \left[ \ln \det(Q + \lambda I_{uv}) \right]_{\lambda=0} = Q_{vu}^{-1}
\]
with \((I_{uv})_{xy} = \delta_{ux}\delta_{vy}\) and variable scalar field was verified numerically, where the left hand side was evaluated by our determinant algorithm and the right hand side with the help of the conjugate gradient algorithm.

4. For particular choices of the Yukawa couplings the determinant has to be real. We checked this property to a high precision.

In all cases the deviations were of the size of the numerical precision of the computer. For example in the last mentioned item the ratio of the imaginary to the real part of the determinant was of the order of 10\(^{-14}\).

### 3 Results on the fermion determinant

Some general results on the fermion determinant in the \(U(1)_L \otimes U(1)_R\) symmetric Yukawa model are available.

1. The expectation value \(\overline{\det Q}\) is real. This is due to \(\overline{\det Q(\phi^+)} = (\overline{\det Q(\phi)})^*\), and the weight of a scalar field \(\phi\) in the functional integral being the same as that of its complex conjugate \(\phi^+\).

2. For \(G_\psi = \pm G_\chi\) the determinant is real for each single scalar field configuration, as can be shown using the symmetries of the action.

For other physically interesting choices of parameters the aim is to obtain information about the size of the fluctuations of the phase angle \(\alpha\) defined by
\[
\det Q = |\det Q| e^{i\alpha}.
\]

We have investigated the fermion determinant in four series of points in the parameter space. Each series is specified by the values of \(G_\psi, G_\chi, K\) and the quartic scalar self-coupling \(\lambda\). The parameters are summarized in table 1. Series D has a real determinant and serves as a check on the program.

Within each series the scalar hopping parameter \(\kappa\) was varied in such a way that five equidistant points in parameter space are obtained, which start in the symmetric phase near a scalar mass of \(m_R \approx 1\) and end in the phase with broken symmetry at a scalar mass of the same magnitude. This covers the physically interesting region near the second order phase transition line. At each of the 20 points in parameter space after equilibration the determinant was calculated 40 times, always separated by hundred trajectories from each other. The results of the calculation are displayed in table 2. It displays the average
values of the real and the imaginary parts of \( \det Q \), together with the average value \( \bar{\alpha} \) of the phase and its standard deviation

\[
\Delta \alpha = \frac{1}{40} \sum_{i=1}^{40} (\alpha_i - \bar{\alpha})^2.
\] (10)

In series D, where the phase is known to be zero, the standard deviation of \( \alpha \) yields an estimate of the precision of the numerical results.

From the data it appears that nothing particular happens to the determinant when the vicinity of the phase transition is passed. The absolute values of both the real and the imaginary parts increase continuously from the symmetric to the broken phase. The average values of \( \alpha \) are always statistically consistent with zero, as they should.

Most important is the observation that in all points the standard deviation of \( \alpha \) is very small. Its value in series A, where it is largest, is near \( 2 \cdot 10^{-3} \). In this series the Yukawa couplings differ most in their absolute values. This represents the case that is farthest from \( G_\psi = \pm G_\chi \), where \( \alpha \) vanishes.

4 Conclusion

The investigation of the complex fermion determinant in the \( U(1)_L \otimes U(1)_R \) symmetric Yukawa model with mirror fermions has shown that the phase of the determinant is fluctuating only very little, while the modulus of the determinant varies over many orders of magnitude in the physically interesting region. Thus a simulation of the model without further technical doubling of the number of fermions appears feasible. This could be achieved by a Hybrid Classical–Langevin algorithm based on the effective action \( S(\phi) - 1/2 \ln \det QQ^+ \).

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Table 1
Parameters of the four series of points at which the fermion determinant has been measured.

| label | $\lambda$ | $G_\psi$ | $G_\chi$ | $K$ |
|-------|-----------|----------|----------|-----|
| A     | 1.0       | 1.0      | 0.0      | 0.10|
| B     | 1.0       | 0.3      | 0.0      | 0.10|
| C     | $10^{-4}$ | 0.1      | -0.2     | 0.13|
| D     | 1.0       | 0.3      | -0.3     | 0.10|

Table 2
Results of the numerical calculation of the complex fermion determinant.

| label | $\kappa$ | Re det $Q$ | Im det $Q$ | $\tau$     | $\Delta \alpha$ |
|-------|----------|-----------|------------|------------|-----------------|
| A     | 0.070    | $6.90 \cdot 10^7$ | $2.68 \cdot 10^4$ | $3.89 \cdot 10^{-4}$ | $2.04 \cdot 10^{-3}$ |
|       | 0.079    | $2.20 \cdot 10^8$  | $-2.48 \cdot 10^5$ | $2.54 \cdot 10^{-5}$ | $2.67 \cdot 10^{-3}$ |
|       | 0.088    | $3.34 \cdot 10^{11}$ | $7.07 \cdot 10^7$  | $-6.17 \cdot 10^{-4}$ | $2.23 \cdot 10^{-3}$ |
|       | 0.097    | $9.65 \cdot 10^{13}$ | $-6.46 \cdot 10^{10}$ | $2.95 \cdot 10^{-4}$ | $2.16 \cdot 10^{-3}$ |
|       | 0.105    | $7.70 \cdot 10^{18}$ | $-2.14 \cdot 10^{15}$ | $-4.11 \cdot 10^{-4}$ | $2.16 \cdot 10^{-3}$ |
| B     | 0.137    | $1.67 \cdot 10^3$  | $4.51 \cdot 10^{-3}$ | $1.15 \cdot 10^{-6}$ | $1.90 \cdot 10^{-5}$ |
|       | 0.145    | $2.03 \cdot 10^3$  | $5.28 \cdot 10^{-4}$ | $5.55 \cdot 10^{-7}$ | $2.24 \cdot 10^{-5}$ |
|       | 0.153    | $2.64 \cdot 10^3$  | $-1.35 \cdot 10^{-2}$ | $-3.55 \cdot 10^{-6}$ | $2.18 \cdot 10^{-5}$ |
|       | 0.160    | $3.09 \cdot 10^3$  | $-2.10 \cdot 10^{-2}$ | $-1.61 \cdot 10^{-6}$ | $2.52 \cdot 10^{-5}$ |
|       | 0.168    | $5.46 \cdot 10^3$  | $-1.98 \cdot 10^{-2}$ | $-2.34 \cdot 10^{-6}$ | $2.14 \cdot 10^{-5}$ |
| C     | 0.077    | $5.72 \cdot 10^{35}$ | $-5.38 \cdot 10^{31}$ | $1.54 \cdot 10^{-5}$ | $1.70 \cdot 10^{-4}$ |
|       | 0.081    | $5.77 \cdot 10^{36}$ | $-1.81 \cdot 10^{33}$ | $-5.58 \cdot 10^{-5}$ | $2.52 \cdot 10^{-4}$ |
|       | 0.086    | $9.24 \cdot 10^{38}$ | $4.56 \cdot 10^{35}$  | $-2.20 \cdot 10^{-5}$ | $2.45 \cdot 10^{-4}$ |
|       | 0.091    | $3.95 \cdot 10^{42}$ | $-2.30 \cdot 10^{38}$ | $-1.16 \cdot 10^{-5}$ | $2.57 \cdot 10^{-4}$ |
|       | 0.096    | $2.20 \cdot 10^{65}$ | $-8.98 \cdot 10^{60}$ | $3.42 \cdot 10^{-5}$  | $1.53 \cdot 10^{-4}$ |
| D     | 0.104    | $3.90 \cdot 10^{84}$ | $-1.39 \cdot 10^{70}$ | $1.81 \cdot 10^{-16}$ | $5.50 \cdot 10^{-15}$ |
|       | 0.109    | $1.10 \cdot 10^{85}$ | $-2.73 \cdot 10^{70}$ | $-7.16 \cdot 10^{-16}$ | $6.53 \cdot 10^{-15}$ |
|       | 0.114    | $3.38 \cdot 10^{86}$ | $2.52 \cdot 10^{72}$  | $9.54 \cdot 10^{-16}$ | $8.06 \cdot 10^{-15}$ |
|       | 0.119    | $2.55 \cdot 10^{88}$ | $-1.02 \cdot 10^{74}$ | $-1.68 \cdot 10^{-16}$ | $7.65 \cdot 10^{-15}$ |
|       | 0.124    | $1.27 \cdot 10^{89}$ | $2.44 \cdot 10^{75}$  | $2.57 \cdot 10^{-15}$ | $7.42 \cdot 10^{-15}$ |