Majorana fermions on the lattice

István Montvay

Deutsches Elektronen-Synchrotron DESY,
Notkestr. 85, D-22603 Hamburg, Germany

Abstract

The Monte Carlo simulation of Majorana fermions is discussed on the example of supersymmetric Yang-Mills (SYM) theory.

1 Introduction

Majorana fermions play an important rôle in supersymmetric quantum field theories which are the favorite candidates for the extension of the Standard Model of elementary particle interactions beyond the presently available energy range. It is generally assumed that the scale where supersymmetry becomes manifest is near to the presently explored electroweak scale and that the supersymmetry breaking is spontaneous. An attractive possibility for spontaneous supersymmetry breaking is to exploit non-perturbative mechanisms in supersymmetric gauge theories.

Non-perturbative features of supersymmetric theories can be derived analytically, as for instance the basic work of Seiberg and Witten [1] shows, and can also be obtained by numerical Monte Carlo simulations on a lattice. The numerical approach requires the introduction of Majorana fermion fields on a four-dimensional Euclidean lattice in space and imaginary time.

The simplest supersymmetric gauge theory is the supersymmetric extension of Yang-Mills gauge theory. It is the gauge theory of a massless Majorana fermion, called “gaugino”, in the adjoint representation of the

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The Euclidean action density of a gauge theory in the adjoint representation can be written as

\[ \mathcal{L} = \frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a + \frac{1}{2} \lambda^a (D_\mu \lambda)^a + m_{\tilde{g}} \overline{\lambda}^a \lambda^a . \]  

(1)

Here \( F_{\mu\nu}^a \) denotes the field strength tensor and \( \lambda^a \) is the Grassmannian fermion field, both with the adjoint representation index \( a \). \( m_{\tilde{g}} \) is the gaugino mass which has to be set equal to zero for supersymmetry. For a Majorana fermion \( \lambda^a \) and \( \overline{\lambda}^a \) are not independent but satisfy

\[ \overline{\lambda} = \lambda^T C , \]  

(2)

with \( C \) the charge conjugation Dirac matrix. This definition is based on the analytic continuation of Green’s functions from Minkowski to Euclidean space \([2]\).

## 2 Lattice formulation

In order to define the path integral for a Yang Mills theory with Majorana fermions in the adjoint representation, let us first consider the familiar case of Dirac fermions \([3]\). (For a general reference on lattice quantum field theory see this book.) Let us denote the Grassmanian fermion fields in the adjoint representation by \( \psi_x^a \) and \( \overline{\psi}_x^a \). Here Dirac spinor indices are omitted for simplicity and \( a \) stands for the adjoint representation index \((a = 1, \ldots, N^2_c - 1 \text{ for } \text{SU}(N_c))\). The fermionic part of the Wilson lattice action is

\[ S_f = \sum_x \left\{ \overline{\psi}_x^a \psi_x^a \right\} - K \sum_{\mu=1}^4 \left[ \overline{\psi}_{x+\mu} V_{ab,x\mu} (1 + \gamma_\mu) \psi_x^b + \overline{\psi}_x V^T_{ab,x\mu} (1 - \gamma_\mu) \psi_{x+\mu}^b \right] . \]  

(3)

Here \( K \) is the hopping parameter, the Wilson parameter removing the fermion doublers in the continuum limit is fixed to \( r = 1 \) and the matrix for the gauge-field link in the adjoint representation \( V_{x\mu} \) is defined from the fundamental link variables \( U_{x\mu} \) according to

\[ V_{ab,x\mu} \equiv V_{ab,x\mu}[U] \equiv 2 \text{Tr}(U_{x\mu}^T T_a U_{x\mu} T_b) = V_{ab,x\mu}^* = V_{ab,x\mu}^{-1T} . \]  

(4)
The generators $T_a \equiv \frac{1}{2} \lambda_a$ satisfy the usual normalization $\text{Tr} (\lambda_a \lambda_b) = \frac{1}{2}$. In the simplest case of SU(2) ($N_c = 2$) we have, of course, $T_a \equiv \frac{1}{2} \tau_a$ with the isospin Pauli-matrices $\tau_a$. The normalization of the fermion fields in (3) is the usual one for numerical simulations. The full lattice action is the sum of the pure gauge part and fermionic part:

$$S = S_g + S_f .$$

The standard Wilson action for the SU($N_c$) gauge field $S_g$ is a sum over the plaquettes

$$S_g = \beta \sum_{pl} \left( 1 - \frac{1}{N_c} \text{Re} Tr U_{pl} \right) ,$$

with the bare gauge coupling given by $\beta \equiv 2N_c / g^2$.

In order to obtain the lattice formulation of a theory with Majorana fermions let us note that out of a Dirac fermion field it is possible to construct two Majorana fields:

$$\lambda^{(1)} \equiv \frac{1}{\sqrt{2}} (\psi + C \psi^T) , \quad \lambda^{(2)} \equiv i \frac{1}{\sqrt{2}} (\psi + C \psi^T)$$

with the charge conjugation matrix $C$. These satisfy the Majorana condition

$$\lambda^{(j)} = \lambda^{(j)T} C \quad (j = 1, 2) .$$

The inverse relation of (7) is

$$\psi = \frac{1}{\sqrt{2}} (\lambda^{(1)} + i \lambda^{(2)}) , \quad \psi_c \equiv C \psi^T = \frac{1}{\sqrt{2}} (\lambda^{(1)} - i \lambda^{(2)}) .$$

In terms of the two Majorana fields the fermion action $S_f$ in eq. (3) can be written as

$$S_f = \frac{1}{2} \sum_{x} \sum_{j=1}^{2} \left\{ \lambda^{(j)a}_x \lambda^{(j)a}_x - K \sum_{\mu=1}^{4} \left[ \lambda^{(j)a}_x V_{ab,x}\mu (1 + \gamma_{\mu}) \lambda^{(j)b}_{x+\mu} + \lambda^{(j)a}_x V^T_{ab,x}\mu (1 - \gamma_{\mu}) \lambda^{(j)b}_{x+\mu} \right] \right\} .$$

For later purposes it is convenient to introduce the fermion matrix

$$Q_{yd,xc} \equiv Q_{yd,xc}[U] \equiv \delta_{yx} \delta_{dc}$$

$$- K \sum_{\mu=1}^{4} \left[ \delta_{y,x+\mu} (1 + \gamma_{\mu}) V_{dc,x}\mu + \delta_{y+\mu,x} (1 - \gamma_{\mu}) V^T_{dc,x}\mu \right] .$$
Here, as usual, \( \hat{\mu} \) denotes the unit vector in direction \( \mu \). In terms of \( Q \) we have

\[
S_f = \sum_{xc,yd} \bar{\psi}_y Q_{yd,xc} \psi_x^c = \frac{1}{2} \sum_{j=1}^{2} \sum_{xc,yd} \lambda^{(j)d}_y Q_{yd,xc} \lambda^{(j)c}_x ,
\]

(12)

and the fermionic path integral can be written as

\[
\int [d\bar{\psi} d\psi] e^{-S_f} = \int [d\bar{\psi} d\psi] e^{-\bar{\psi} Q \psi} = \det Q = \prod_{j=1}^{2} \int [d\lambda^{(j)}] e^{-\frac{1}{4} \lambda^{(j)} Q \lambda^{(j)}} .
\]

(13)

This shows that the path integral over the Dirac fermion is the square of the path integral over the Majorana fermion and therefore

\[
\int [d\lambda] e^{-\frac{1}{4} \lambda Q \lambda} = \pm \sqrt{\det Q} .
\]

(14)

As one can see here, for Majorana fields the path integral involves only \([d\lambda^{(j)}]\) because of the Majorana condition in (8).

The relation (14) leaves the sign on the right hand side undetermined. A unique definition of the path integral over a Majoran fermion field, including the sign, is given by

\[
\int [d\lambda] e^{-\frac{1}{4} \lambda Q \lambda} = \int [d\lambda] e^{-\frac{1}{4} \lambda M \lambda} = \text{Pf}(M)
\]

(15)

where \( M \) is the antisymmetric matrix defined as

\[
M \equiv C Q = -M^T .
\]

(16)

The square root of the determinant in eq. (14) is a Pfaffian \[\text{Pf}\]. This can be defined for a general complex antisymmetric matrix \( M_{\alpha \beta} = -M_{\beta \alpha} \) with an even number of dimensions \( (1 \leq \alpha, \beta \leq 2N) \) by a Grassmann integral as

\[
\text{Pf}(M) \equiv \int [d\phi] e^{-\frac{1}{2} \phi M \phi} = \frac{1}{N! 2^N \epsilon_{\alpha_1 \beta_1 \ldots \alpha_N \beta_N}} M_{\alpha_1 \beta_1} \ldots M_{\alpha_N \beta_N} .
\]

(17)

Here, of course, \([d\phi] \equiv d\phi_{2N} \ldots d\phi_1\), and \( \epsilon \) is the totally antisymmetric unit tensor.

It is now clear that the fermion action for a Majorana fermion in the adjoint representation \( \lambda^a_x \) can be defined by

\[
S_f \equiv \frac{1}{2} \lambda Q \lambda = \frac{1}{2} \sum_x \left\{ \lambda^a_x \lambda^a_x \right\} - K \sum_{\mu=1}^{4} \left[ \lambda^a_{x+\hat{\mu}} V_{ab,x+\mu}(1 + \gamma_\mu) \lambda^b_x + \lambda^a_x V^T_{ab,x+\mu}(1 - \gamma_\mu) \lambda^b_{x+\hat{\mu}} \right] .
\]

(18)
This together with (5)-(6) gives a lattice action for the gauge theory of Majorana fermion in the adjoint representation. In order to achieve supersymmetry one has to tune the hopping parameter (bare mass parameter) \( K \) to the critical value \( K_{cr}(\beta) \) in such a way that the mass of the fermion becomes zero.

The path integral over \( \lambda \) is defined by the Pfaffian \( \text{Pf}(CQ) = \text{Pf}(M) \). By this definition the sign on the right hand side of eq. (14) is uniquely determined. The determinant \( \det(Q) \) is real because the fermion matrix in (11) satisfies

\[
Q^\dagger = \gamma_5 Q \gamma_5 , \quad \bar{Q} \equiv \gamma_5 Q = \bar{Q}^\dagger .
\]  

Moreover one can prove that \( \det(Q) = \det(\bar{Q}) \) is always non-negative. This follows from the relations

\[
CQC^{-1} = Q^T , \quad B\bar{Q}B^{-1} = \bar{Q}^T ,
\]

with the charge conjugation matrix \( C \) and \( B \equiv C\gamma_5 \). It follows that every eigenvalue of \( Q \) and \( \bar{Q} \) is (at least) doubly degenerate. Therefore, with the real eigenvalues \( \tilde{\lambda}_i \) of the Hermitean fermion matrix \( \bar{Q} \), we have

\[
\det(Q) = \det(\bar{Q}) = \prod_i \tilde{\lambda}_i^2 \geq 0 .
\]  

Since according to the above discussion

\[
\det(Q) = \det(M) = [\text{Pf}(M)]^2 ,
\]

the Pfaffian \( \text{Pf}(M) \) has to be real – but it can have any sign.

3 Numerical simulations of SYM theories

In order to perform Monte Carlo simulations of SYM theory one needs a positive measure on the gauge field which allows for importance sampling of the path integral. Therefore the sign of the Pfaffian can only be taken into account by reweighting. According to (22) the absolute value of the Pfaffian is the non-negative square root of the determinant therefore the effective gauge field action is [5]:

\[
S_{CV} = \beta \sum_{pl} \left( 1 - \frac{1}{2} \text{Tr} U_{pl} \right) - \frac{1}{2} \log \det Q[U] .
\]  

(23)
The factor $\frac{1}{2}$ in front of $\log \det Q$ shows that we effectively have a flavour number $N_f = \frac{1}{2}$ of adjoint fermions. The omitted sign of the Pfaffian can be taken into account by reweighting the expectation values according to

$$\langle A \rangle = \frac{\langle A \sign\Pf(M) \rangle_{CV}}{\langle \sign\Pf(M) \rangle_{CV}}, \quad (24)$$

where $\langle \ldots \rangle_{CV}$ denotes expectation values with respect to the effective gauge action $S_{CV}$. This may give rise to a sign problem which will be discussed in section 3.1.

The fractional power of the determinant corresponding to (23) can be reproduced, for instance, by the hybrid molecular dynamics algorithm [6] which is, however, a finite step size algorithm where the step size has to be extrapolated to zero. An “exact” algorithm where the step size extrapolation is absent is the two-step multi-bosonic (TSMB) algorithm [7, 8]. The first large scale numerical simulation of SYM theory has recently been performed by the DESY-Münster-Roma collaboration using the TSMB algorithm [8, 10, 11].

3.1 The “sign problem”

The Pfaffian resulting from the Grassmannian path integrals for Majorana fermions (15) is an object similar to a determinant but less often used. As shown by (17), $\Pf(M)$ is a polynomial of the matrix elements of the $2N$-dimensional antisymmetric matrix $M = -M^T$. Basic relations are [4]

$$M = P^TJ P, \quad \Pf(M) = \det(P), \quad (25)$$

where $J$ is a block-diagonal matrix containing on the diagonal $2 \otimes 2$ blocks equal to $\epsilon = i\sigma_2$ and otherwise zeros. Let us note that from these relations the second equality in eq. (22) immediately follows.

The form of $M$ required in (25) can be achieved by a procedure analogous to the Gram-Schmidt orthogonalization and, by construction, $P$ is a triangular matrix (see [10]). This gives a numerical procedure for the computation of $P$ and the determinant of $P$ gives, according to (25), the Pfaffian $\Pf(M)$. Since $P$ is triangular, the calculation of $\det(P)$ is, of course, trivial.

This procedure can be used for a numerical determination of the Pfaffian on small lattices. On lattices larger than, say, $4^3 \cdot 8$ the computation
becomes cumbersome due to the large storage requirements. This is because one has to store a full $\Omega \otimes \Omega$ matrix, with $\Omega$ being the number of lattice points multiplied by the number of spinor-colour indices (equal to $4(N_c^2 - 1)$ for the adjoint representation of $SU(N_c)$). The difficulty of computation is similar to a computation of the determinant of $Q$ with $LU$-decomposition.

Fortunately, in order to obtain the sign of the Pfaffian occurring in the reweighting formula (27), one can proceed without a full calculation of the value of the Pfaffian. The method is to monitor the sign changes of $\text{Pf}(M)$ as a function of the hopping parameter $K$. According to (21), the hermitean fermion matrix for the gaugino $\tilde{Q}$ has doubly degenerate real eigenvalues therefore

$$\det M = \det \tilde{Q} = \prod_{i=1}^{\Omega/2} \tilde{\lambda}_i^2,$$  \hspace{1cm} (26)

where $\tilde{\lambda}_i$ denotes the eigenvalues of $\tilde{Q}$. This implies

$$|\text{Pf}(M)| = \prod_{i=1}^{\Omega/2} |\tilde{\lambda}_i|, \quad \implies \quad \text{Pf}(M) = \prod_{i=1}^{\Omega/2} \tilde{\lambda}_i.$$  \hspace{1cm} (27)

The first equality trivially follows from (22). The second one is the consequence of the fact that $\text{Pf}(M)$ is a polynomial in $K$ which cannot have discontinuities in any of its derivatives. Therefore if, as a function of $K$, an eigenvalue $\tilde{\lambda}_i$ (or any odd number of them) changes sign the sign of $\text{Pf}(M)$ has to change, too. Since at $K = 0$ we have $\text{Pf}(M) = 1$, the number of sign changes between $K = 0$ and the actual value of $K$, where the dynamical fermion simulation is performed, determines the sign of $\text{Pf}(M)$. This means that one has to determined the flow of the eigenvalues of $\tilde{Q}$ through zero [12].

The spectral flow method is well suited for the calculation of the sign of the Pfaffian in SYM theory. An important question is the frequency and the effects of configurations with negative sign. A strongly fluctuating Pfaffian sign is a potential danger for the effectiveness of the Monte Carlo simulation because cancellations can occur resulting in an unacceptable increase of statistical errors. The experience of the DESY-Münster Collaboration shows, however, that below the critical line $K_{cr}(\beta)$ corresponding to zero gaugino mass ($m_{\tilde{g}} = 0$) negative Pfaffians practically never appear.
Above the critical line several configurations with negative Pfaffian have been observed but their rôle has not yet been cleared up to now. Since supersymmetry is expected to be realized in the continuum limit at $m_{\tilde{g}} = 0$, the negative signs of the Pfaffian can be avoided if one takes the zero gaugino mass limit from $m_{\tilde{g}} > 0$ corresponding to $K < K_{cr}$. In this sense there is no “sign problem” in SYM which would prevent a Monte Carlo investigation.

The presence or absence of negative Pfaffians in a sample of gauge configurations produced in Monte Carlo simulations can be easily seen even without the application of the spectral flow method. In case of sign changes the distribution of the smallest eigenvalues of the squared fermion matrix $\tilde{Q}^2$ shows a pronounced tail reaching down to zero [13]. The absence of a tail shows that there are no negative Pfaffians.

Concerning this “sign problem” let us note that a very similar phenomenon appears also in QCD because the Wilson-Dirac determinant of a single quark flavour can also have a negative sign. Under certain circumstances the sign of the quark determinant plays an important rôle. This is the case, for instance, at large quark chemical potential in a QCD-like model with SU(2) colour and staggered quarks in the adjoint representation which has recently been studied by the DESY-Swansea Collaboration [13]. This investigation also revealed an interesting feature of the TSMB algorithm, namely its ability to easily change the sign of eigenvalues of the hermitean fermion matrix (and hence the sign of the determinant or Pfaffian). This is in contrast to algorithms based on finite difference molecular dynamics equations as, for instance, the HMD [6] algorithms.

4 Outlook

Numerical simulations of $N = 1$ supersymmetric theories require to deal with Majorana fermions on a Euclidean lattice. Such simulations are feasible with presently available computer technology and using well established simulation algorithms – at least in the relatively simple case of supersymmetric Yang-Mills theories [3, 10, 11, 14, 15]. Many interesting questions are waiting for detailed answers. Just to mention a few: the behaviour of the phase transition at the supersymmetric point, the spectroscopy of supersymmetric multiplets in the particle spectrum and the Ward-Takahashi identities proving the realization of supersymmetry
in quantum field theories.

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