1 Towards the lattice simulation

With the current status of the action (??) we could almost start to discretize the operators and fields, at least for the bosonic part this would not be a problem. For the fermions however this is not so straight forward. In order to include the fermionic contribution into the weight factor of the path integral like explained in section ?? one needs to integrate out the GRASS-MANN variables to result into a PFAFFIAN or determinant of a fermionic operator. As presented in Appendix ?? this is only possible if the fermions appearing are of quadratic order. But in the fluctuation action (??) also quartic contributions of fermions appear, which have to be linearized with help of a Hubbard-Statonovich transformation.¹

1.1 Linearization of fermionic contributions

1.1.1 Naive approach and sign problem

The only quartic interactions are coming from the η fields and we can write this part of the action as

$$S_4^{\mathrm{F}}[\eta_i, \eta^i] = g \int dt ds \left[-\frac{1}{z^2} (\eta^2)^2 + \left(\frac{i}{z^2} z_N \eta_i (\rho^{MN})^i_{\ j} \eta^j \right)^2 \right].$$
 (1.1)

In the path integral representation the euclidean action contributes within an exponential e^{-S_E} . By performing a naive Hubbard-Statonovich transformation to this exponential we can reduce the four-fermion contributions to quadratic Yukawa terms whereas we have to introduce 7 bosonic real auxiliary fields ϕ and ϕ^N

$$\exp\left\{-g\int dtds \left[-\frac{1}{z^{2}}(\eta^{2})^{2} + \left(\frac{i}{z^{2}}z_{N}\eta_{i}(\rho^{MN})^{i}_{j}\eta^{j}\right)^{2}\right]\right\}$$

$$\sim \int \mathcal{D}\phi\mathcal{D}\phi^{\mathcal{M}} \exp\left\{-g\int dtds \left[\frac{1}{2}\phi^{2} + \frac{\sqrt{2}}{z}\phi\eta^{2} + \frac{1}{2}(\phi^{M})^{2} - i\frac{\sqrt{2}}{z^{4}}\phi_{M}\left(i\eta_{i}(\rho^{MN})^{i}_{j}\eta^{j}\right)z_{N}\right]\right\}.$$

$$\left. -i\frac{\sqrt{2}}{z^{4}}\phi_{M}\left(i\eta_{i}(\rho^{MN})^{i}_{j}\eta^{j}\right)z_{N}\right]\right\}.$$

$$\left. -i\frac{\sqrt{2}}{z^{4}}\phi_{M}\left(i\eta_{i}(\rho^{MN})^{i}_{j}\eta^{j}\right)z_{N}\right]\right\}.$$

Here we can notice that the second term appears to be complex, since the SO(6) matrix in parenthesis is hermitian (with respect to the indices M, N)

$$\left(i\eta_i(\rho^{MN})^i_{\ j}\eta^j\right)^{\dagger} = i\eta_j(\rho^{MN})^i_{\ i}\eta^i,\tag{1.3}$$

where we have used (??). As discussed in section ?? this complex phase in the weight function is potentially leading to a non treatable sign problem. We therefore chose to make a field redefinition that circumvents the appearance of a complex phase during the HS transformation.

¹See Appendix ?? for details

1.1.2 Alternative field redefinition

By using the identities for the SO(6) matrices stated in Appendix ?? we can rewrite the second term in the LAGGRANGIAN of (1.1) as

$$\left(i\eta_{i}(\rho^{MN})^{i}_{j}n^{N}\eta^{j}\right)^{2} = -3(\eta^{2})^{2} + 2\eta_{i}(\rho^{N})^{ik}n_{N}\eta_{k}\eta^{j}(\rho^{L})_{jl}n_{L}\eta^{l}, \qquad (1.4)$$

where we defined $n^N = \frac{z^N}{z}$. This leads to the LAGRANGIAN

$$\mathcal{L}_{4} = \frac{1}{z^{2}} \left(-4 \left(\eta^{2} \right)^{2} + 2 \left| \eta_{i} (\rho^{N})^{ik} n_{N} \eta_{k} \right|^{2} \right). \tag{1.5}$$

In order to circumvent the sign problem the second term needs to be negative. To achieve this we define new fields²

$$\Sigma_i^j = \eta_i \eta^j \qquad \tilde{\Sigma}_i^i = (\rho^N)^{ik} n_N (\rho^L)_{jl} n_L \eta_k \eta^l. \tag{1.6}$$

with this new definitions it is simple to check that

$$\Sigma_i^j \Sigma_j^i = -(\eta^2)^2 \qquad \tilde{\Sigma}_i^j \tilde{\Sigma}_j^i = -(\eta^2)^2 \qquad \Sigma_j^i \tilde{\Sigma}_i^j = -\left|\eta_i(\rho^N)^{ik} n_N \eta_k\right|^2. \tag{1.7}$$

With this we now define

$$\Sigma_{\pm i}^{\ j} = \Sigma_i^j \pm \tilde{\Sigma}_i^j \tag{1.8}$$

and find

$$\Sigma_{\pm i}^{j} \Sigma_{\pm j}^{i} = -2(\eta^{2})^{2} \mp 2 \left| \eta_{i}(\rho^{N})^{ik} n_{N} \eta_{k} \right|^{2}. \tag{1.9}$$

We can now substitute the new fields into the LAGRANGIAN and obtain

$$\mathcal{L}_4 = \frac{1}{2} \left(-4 (\eta^2)^2 \mp 2(\eta^2)^2 \mp \sum_{i=1}^{j} \sum_{i=1}^{i} \right) , \qquad (1.10)$$

where we only need to select the right sign in the field definition to overcome the sign problem, which is leading to

$$\mathcal{L}_4 = \frac{1}{r^2} \left(-6 \left(\eta^2 \right)^2 - \Sigma_{+i}^{\ j} \Sigma_{+j}^{\ i} \right) . \tag{1.11}$$

If we now perform a HS transformation there will be no complex phase. The HS transformation yields

$$-\frac{6}{z^2}(\eta^2)^2 \to \frac{12}{z}\eta^2\phi + 6\phi^2,\tag{1.12}$$

where a single bosonic field was introduced like in the naive case. And further

$$-\frac{1}{z^2} \Sigma_{+j}^{i} \Sigma_{+i}^{j} \to \frac{2}{z} \Sigma_{+j}^{i} \phi_i^j + \phi_j^i \phi_i^j \quad \text{with} \quad (\phi_j^i)^* = \phi_i^j . \tag{1.13}$$

Here the collection of fields ϕ_j^i can be thought of as a complex hermitian matrix with 16 real free parameters. We find it convenient to rescale the

²Where we actually set $\Sigma_i^j = \eta_i \eta^j$, then defined $\Sigma^i{}_j \equiv (\Sigma_i^j)^* = \Sigma_j^i$ to emphasize the notation Σ^j_i and equivalent for $\tilde{\Sigma}$.

field $\phi \to \phi/\sqrt{6}$, to get rid of the pre factor of 6 in (1.12). After reinserting the old fields for Σ_+ we can conclude that

$$\mathcal{L}_4 \to \frac{12}{z} \eta^2 \phi + \phi^2 + \frac{2}{z} \eta_j \phi_i^j \eta^i + \frac{2}{z} (\rho^N)^{ik} n_N \eta_k \phi_i^j (\rho^L)_{jl} n_L \eta^l + \phi_j^i \phi_i^j . \quad (1.14)$$

So now we can write the full LAGRANGIAN as

$$\mathcal{L}_{\text{cusp}} = \left| \partial_t x + \frac{m}{2} x \right|^2 + \frac{1}{z^4} \left| \partial_s x - \frac{m}{2} x \right|^2 + \left(\partial_t z^M + \frac{m}{2} z^M \right)^2$$

$$+ \frac{1}{z^4} \left(\partial_s z^M - \frac{m}{2} z^M \right)^2 + \phi^2 + \text{Tr} \left(\tilde{\phi} \, \tilde{\phi}^{\dagger} \right) + \Psi^T \mathcal{O}_F \Psi .$$
(1.15)

Hereby we defined the fermionic vector $\Psi \equiv (\theta^i, \theta_i, \eta^i, \eta_i)$ as well as the auxiliary matrix $\tilde{\phi} = (\tilde{\phi}_{ij}) \equiv \phi^i_j$. We used partial integration and the properties of the Grassmann numbers and SO(6) matrices to write the fermionic contribution in a matrix-vector notation. The 16×16 fermionic operator is hereby represented as 4×4 block matrix

$$\mathcal{O}_{F} = \begin{pmatrix}
0 & i\mathbb{1}_{4}\partial_{t} & -i\rho^{M}\left(\partial_{s} + \frac{m}{2}\right)\frac{z^{M}}{z^{3}} & 0 \\
i\mathbb{1}_{4}\partial_{t} & 0 & 0 & -i\rho_{M}^{\dagger}\left(\partial_{s} + \frac{m}{2}\right)\frac{z^{M}}{z^{3}} \\
i\frac{z^{M}}{z^{3}}\rho^{M}\left(\partial_{s} - \frac{m}{2}\right) & 0 & 2\frac{z^{M}}{z^{4}}\rho^{M}\left(\partial_{s}x - m\frac{x}{2}\right) & i\mathbb{1}_{4}\partial_{t} - A^{T} \\
0 & i\frac{z^{M}}{z^{3}}\rho_{M}^{\dagger}\left(\partial_{s} - \frac{m}{2}\right) & i\mathbb{1}_{4}\partial_{t} + A & -2\frac{z^{M}}{z^{4}}\rho_{M}^{\dagger}\left(\partial_{s}x^{*} - m\frac{x}{2}^{*}\right)
\end{pmatrix},$$
(1.16)

where

$$A = -\frac{\sqrt{6}}{z}\phi \mathbb{1}_4 + \frac{1}{z}\tilde{\phi} + \frac{1}{z^3}\rho_N^*\tilde{\phi}^T\rho^L z^N z^L + i\frac{z^N}{z^2}\rho^{MN}\partial_t z^M.$$
 (1.17)

The auxiliary matrix $\tilde{\phi}$ is constructed from 16 real auxiliary fields ϕ_I ($I = 1, \ldots, 16$) in the following way

$$\tilde{\phi} = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2}\phi_{13} & \phi_1 + i\phi_2 & \phi_3 + i\phi_4 & \phi_5 + i\phi_6 \\ \phi_1 - i\phi_2 & \sqrt{2}\phi_{14} & \phi_7 + i\phi_8 & \phi_9 + i\phi_{10} \\ \phi_3 - i\phi_4 & \phi_7 - i\phi_8 & \sqrt{2}\phi_{15} & \phi_{11} + i\phi_{12} \\ \phi_5 - i\phi_6 & \phi_9 - i\phi_{10} & \phi_{11} - i\phi_{12} & \sqrt{2}\phi_{16} \end{pmatrix}, \tag{1.18}$$

so that we have the simple expression for

$$\operatorname{Tr}\left(\tilde{\phi}\,\tilde{\phi}^{\dagger}\right) = \sum_{I=1}^{16} (\phi_I)^2 \equiv (\phi_I)^2. \tag{1.19}$$

1.1.3 Pseudofermionic weight function

Now since we have linearised fermionic contributions to quadratic order, we are able to integrate over the Grassmann fields in the partition function

$$Z = \int \mathcal{D}x \, \mathcal{D}x^* \, \mathcal{D}z^N \, \mathcal{D}\phi \, \mathcal{D}\phi_I \, \mathcal{D}\Psi \, e^{-S} \,, \tag{1.20}$$

where we will split $S = S_B + S_F$ into its bosonic (S_B) and fermionic (S_F) contributions with

$$S_{\rm B} = g \int dt ds \left| \partial_t x + \frac{m}{2} x \right|^2 + \frac{1}{z^4} \left| \partial_s x - \frac{m}{2} x \right|^2 + \left(\partial_t z^M + \frac{m}{2} z^M \right)^2 + \frac{1}{z^4} \left(\partial_s z^M - \frac{m}{2} z^M \right)^2 + \phi^2 + (\phi_I)^2,$$
(1.21)

$$S_{\rm F} = g \int \mathrm{d}t \mathrm{d}s \ \Psi^T \mathcal{O}_{\rm F} \Psi \,.$$

As motivated in section ?? the Grassmann integral over Ψ will result in a PFAFFIAN Pf \mathcal{O}_{F} . To include the PFAFFIAN into the weight function we have to rewrite it in terms of pseudofermions ξ as emphasized in section ??. To legitimately apply this procedure we need the PFAFFIAN to be real and non-negative. By our alternative approach to linearization we made sure to exclude any potential phase ambiguities. All terms in the action $S_{\rm F}$ are real and therefore also the PFAFFIAN turns out to be a real quantity. So the only problem that we might have to face is if the PFAFFIAN is negative. We would need to be able to write the PFAFFIAN as a perfect square of another quantity to show that it is real for all configurations. We could not show this to be the case analytically (except for some special cases) but there are some hints that point out for this to be legitimate to assume. First of all it can be observed numerically that the PFAFFIAN is always positive at least for large values of g and second also the eigenvalue spectrum of the fermion matrix suggests this, but we will postpone this argument to a later point when we have discretized the operator \mathcal{O}_{F} . For now we will assume a positive Pfaffian for all situations and make this more legitimate by keeping track of it during simulations. For this reason, we proceed as in [?] and introduce pseudofermions ξ via

$$\int \mathcal{D}\Psi \ e^{-S_{\mathrm{F}}} = \mathrm{Pf} \ \mathcal{O}_{\mathrm{F}} = \left(\det \mathcal{O}_{\mathrm{F}} \ \mathcal{O}_{\mathrm{F}}^{\dagger}\right)^{\frac{1}{4}} = \int \mathcal{D}\xi \ \mathcal{D}\xi^{\dagger} \ e^{-S_{\xi}} \ , \tag{1.22}$$

where

$$S_{\xi} = g \int dt ds \, \xi^{\dagger} \left(\mathcal{O}_{F} \, \mathcal{O}_{F}^{\dagger} \right)^{-\frac{1}{4}} \xi \,, \tag{1.23}$$

and ξ is a collection of 16 complex bosonic scalar fields. But before we can go any further we need to discretize the action with help of the methods introduced in ??.

1.2 Discretizing the action

In the previous steps we have constructed a LAGRANGIAN fitting to our problem and modified terms to be able to apply a RHMC algorithm. To proceed with this task we need a discretized version of the bosonic action and the fermionic operator \mathcal{O}_{F} . For the bosonic term this is quite easy. First we need to do a dimensional analysis of the fields in the action. In

the simulation we can only deal with dimensionless fields. Since the action also needs to be dimensionless we can see that the fields x, x^* and z^M are dimensionless as preferred but the auxiliary fields are of dimension $[\phi] = 1/[a]$. We therefore do a redefinition of these fields

$$a\phi \to \phi,$$
 $a\phi_I \to \phi_I$ (1.24)

in order to have dimensionless quantities as well. We can now write the discretized version of the bosonic action in (??) as

$$S_{\rm B} = g \sum_{n \in \Lambda} \left[\left| x(n+\hat{0}) + \left(\frac{M}{2} - 1 \right) x(n) \right|^2 + \frac{1}{[z(n)]^4} \left| x(n+\hat{1}) - \left(\frac{M}{2} + 1 \right) x(n) \right|^2 + \sum_{M=1}^6 \left\{ \left(z^M(n+\hat{0}) + \left(\frac{M}{2} - 1 \right) z^M(n) \right)^2 + \frac{1}{[z(n)]^4} \left(z^M(n+\hat{1}) - \left(\frac{M}{2} + 1 \right) z^M(n) \right)^2 \right\} + \phi^2(n) + \sum_{I=1}^{16} \left[\phi_I(n) \right]^2 \right]$$

$$(1.25)$$

References