Hubbard Model with Lüscher fermions

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First applications of the new algorithm simulating dynamical fermions are reported. The method reproduces previous results obtained with different techniques.

1. DYNAMICAL FERMIONS AND LÜSCHER REPRESENTATION

The problem of dynamical fermions, even though solved in principle, still provides the considerable challenge in practice. Existing exact algorithms require huge computing resources due to the strong correlations between generated configurations \[1\]. Therefore the recent proposal of Lüscher has attracted a lot of interest \[2,3\]. To remind, the main difficulty with simulating the theory with dynamical fermions consists of the nonlocality of the fermionic determinant

\[
\int [d\Psi d\overline{\Psi}] \exp (-\overline{\Psi} M \Psi) \sim \det(M),
\]

which depends functionally on the gauge field in the case of QCD for example. The local and positive representation for the positive powers of \(\det(M)\) was not found up to date. Lüscher method exploits the well known fact that the inverse of the determinant has such a representation in terms of the standard bosonic fields. He therefore proposes to use the polynomial approximation of the reciprocal function

\[
\frac{1}{s} = \lim_{N \to \infty} P_N(s).
\]

In the simplest case \(P_N(s)\) can be taken as the geometrical series (in \(1 - s\)), in practice better choices are known. Decomposing \(P_N\) into the product form and using the symmetries of roots of real polynomials Lüschler proves that the partition function of the full QCD with two flavours of dynamical quarks has positive and local representation in terms of the original gauge fields and \(N\) bosonic fields associated with zeros of \(P_N(s)\).

It remains now to be tested if this elegant trick is also advantageous in practice. In particular the crucial question is: how do the parameters of this representation scale with the volume and with the bare parameters of the original theory in its critical region? All these important and critical problems are being now thoroughly checked \[4\].

In this contribution I report on the first results of applying the Lüscher’s method to the (Euclidean) three-dimensional Hubbard model, which is the convenient and nontrivial testing ground of the new techniques dealing with dynamical fermions.

2. THE HUBBARD MODEL AND ITS BOSONIC REPRESENTATION

The Hubbard model is a many-body theory of nonrelativistic electrons with the nonlinear point-like coupling representing the effective Coulomb interactions \[5,6\]. Its particular Euclidean formulation contains also the continuous Hubbard-Stratonovich field which couples to the electrons, hence may be regarded as analogous to the Yang-Mills fields of QCD. Even though the nonrelativistic, the model contains all the numerical dif-
ficulties caused by the fermionic statistics, i.e. by the Pauli exclusion principle. Being simpler than QCD it still describes interesting physics of a non-trivial many-body system.

Hubbard Hamiltonian may be written as

\[ H = -K \sum_{<ij>} a_{i\sigma}^\dagger a_{j\sigma} - \frac{U}{2} \sum_i (n_{i\uparrow} - n_{i\downarrow})^2 + \mu \sum_i n_{i\sigma}, \]

where \( n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma} \), and \( a_{i\sigma} \) denotes the creation operator of an electron at the lattice site \( i \) and with the spin \( \sigma = \uparrow, \downarrow \). \( K, U \) and \( \mu \) are the hopping parameter, coupling constant and the chemical potential respectively. Standard transfer matrix formalism gives the following Euclidean representation for the partition function \([7]\):

\[ Z = \int [dA] \exp \left( -\sum_{i,t} A_{it}^2 / 2 \right) \det M_+ \det M_- \]

where the continuous Hubbard-Stratonovich field \( A_{it} \) was introduced to decouple the quartic interaction term. The discrete index \( t = 1, \ldots, N_t \) labels the time slices. Fermionic matrices \( M_{\pm} \) define the bilinear fermionic actions

\[ \Psi^\dagger M_{\pm} \Psi = \frac{K \beta}{N_t} \sum_{<ij,t>} \Psi_{ij}^\dagger \Psi_{it} + \sum_{it} \Psi_{it}^\dagger (\Psi_{it} - \Psi_{it-1}) + \sum_{it} \Psi_{it}^\dagger \Psi_{it} \left( \exp \left[ \frac{U \beta}{N_t} A_{it} - (U \pm \mu) \frac{\beta}{N_t} \right] - 1 \right). \]

At \( \mu = 0 \), which corresponds to the half-filling, \( \det M_+ \det M_- = \det M^2 = \det M \dagger M \),

because the determinants are real. We can therefore apply the Lüscher trick and write the polynomial approximation for the inverse

\[ \frac{1}{Q^\dagger Q} = P_{2N}(Q^\dagger Q) = \prod_{k=1}^{2N} (Q^\dagger Q - z_k) = \prod_{k=1}^{N} (Q^\dagger Q - \alpha_k - i \beta_k)(Q^\dagger Q - \alpha_k + i \beta_k), \]

since the roots \( z_k \equiv \alpha_k + i \beta_k \) of the polynomial \( P_{2N}(z) \) exist in the complex conjugate pairs. \( Q^\dagger Q = M^\dagger M / \lambda_{\text{max}} \) with \( \lambda_{\text{max}} \) being the largest eigenvalue of \( M^\dagger M \).

We therefore have the local and positive representation for the partition function of the Hubbard model.

\[ Z \simeq \int [dA d\phi] \exp \left( -\int A^2(x) / 2 d^3 x \right) \exp \left( -\int \sum_{k=1}^{N} \phi_k^\dagger [(Q^\dagger Q - \alpha_k)^2 + \beta_k^2] \phi_k d^3 x \right) \]

where we have used continuous notation for simplicity. Hence the original system of nonlinearly interacting fermions was replaced by \( N \) complex bosonic fields coupled to the single real scalar field \( \lambda(x) \). This can be simulated with the standard local Monte Carlo techniques. Compared to the original Lüscher mapping we have half as many fields \( \phi_k(x) \), however our bosonic action is more complicated since \( Q^\dagger Q \) contains also next-to-nearest-neighbour interactions.

**2.1. IMPLEMENTATION AND RESULTS**

Convergence of the polynomial approximation, Eq.\( (4) \), cannot be uniform in \( s \) in the whole interval \( (0,1) \). Hence Lüscher introduces the cut-off \( \epsilon > 0 \) such that the series \( (4) \) is uniformly convergent for \( \epsilon < s < 0 \). This parameter enters directly into the construction of the optimal polynomials \( P_N \). The value of \( \epsilon \) is crucial for the practical applicability of the algorithm since it controls the number of bosonic fields required to reach the prescribed accuracy. Ideally \( \epsilon \) should be smaller that the smallest eigenvalue of the normalized matrix \( Q^\dagger Q \). Otherwise corrections for a few eigenvalues lower than \( \epsilon \) could be implemented \( (5) \).

Our preliminary simulations were done on the \( 5^3 \) lattice at \( K = 1 \) and \( U = 1 \). These parameters were chosen to allow comparison with the earlier Creutz results obtained with different algorithm \( (6) \). One Monte Carlo sweep consisted of the heatbath generation of all fields \( \phi_k \) and the Metropolis update of the Hubbard-Stratonovich field \( \lambda(x) \). Fig. 1 shows the distribution of the minimal eigenvalue of \( Q^\dagger Q \). On this basis we have chosen \( \epsilon = 0.001 \). The number of auxiliary fields
$\phi_k$ was fixed to $N = 100$. This guaranteed that the relative error introduced by finite $N$ in Eq.(2) was smaller than $10^{-4}$ for $\epsilon < s$. Instead of $\lambda_{max}$ needed to define the normalized matrix $Q$ we have used the upper bound $\overline{\lambda}$ which can be readily derived

$$\lambda_{max} < 2[\lambda_{max}(A^\dagger A) + max(D)^2] \equiv \overline{\lambda},$$  \hspace{1cm} (10)$$

where $D$ is the diagonal part of $\mathcal{M} = A + D$. Hubbard-Stratonovich field was cut-off by $A(x) < 4$ which would correspond to the four standard deviations if the determinants were neglected. This bound was never violated in practice. Fig. 2 shows the history of the density of the electrons $n_\uparrow$ and of the local number of pairs $n_\uparrow(x) n_\downarrow(x)$. Both observables stabilize relatively quickly and the equilibrium averages agree with the results quoted by Creutz for slightly bigger lattice. For the $6^2 \times 8$ lattice we obtain $< n_\uparrow > = 0.47(3)$ and $< n_\uparrow n_\downarrow > = 0.220(3)$ while the corresponding numbers read from the Creutz plots are 0.48 and 0.22 with the read-out error $\sim 0.01$. The run summarized in Fig. 2 took about 10 hrs of the HP-720.

We have found however that the configurations generated by this algorithm are strongly correlated. The autocorrelation time measured on both densities is approximately 100 sweeps. Similar phenomenon was also reported at this Conference by Jegerlehner while testing QCD implementation.

In conclusion, the Hubbard Model is in the Lüscher class, i.e. it can be mapped onto a system of bosons with local interactions. The half-filled case has a positive Boltzman factor which admits standard Monte Carlo approach. Further studies are needed to investigate whether the large autocorrelation times can be eliminated.

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