Bosonization and Cluster Updating of Lattice Fermions

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Abstract

A lattice fermion model is formulated in Fock space using the Jordan-Wigner representation for the fermion creation and annihilation operators. The resulting path integral is a sum over configurations of lattice site occupation numbers \( n(x, t) = 0, 1 \) which may be viewed as bosonic Ising-like variables. However, as a remnant of Fermi statistics a nonlocal sign factor arises for each configuration. When this factor is included in measured observables the bosonic occupation numbers interact locally, and one can use efficient cluster algorithms to update the bosonized variables.

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Numerical simulations of lattice fermions are important both in particle and in condensed matter physics. For example, in particle physics one simulates quarks to investigate if nonperturbative QCD is the correct theory of strong interactions. In condensed matter physics one simulates electrons to test if the Hubbard model and its variants describe high $T_c$ superconductivity. In both cases it is common to integrate out the fermions. The resulting bosonic effective theories have nonlocal interactions due to the fermion determinant. Because of the nonlocality the theory is not really bosonized, and its numerical simulation is computationally difficult and very time consuming. Of course, one could include the fermion determinant in measured observables and view the system as a local bosonic theory. In practice, however, this does not work because the fermion determinant varies over many orders of magnitude thus making a numerical simulation extremely inefficient.

Jordan and Wigner were the first to realize that fermions can be represented by bosonic operators [1]. Their observation was applied to numerical simulations of fermionic systems in $1 + 1$ dimensions [2]. The resulting path integral is a sum over configurations of occupation numbers $n(x, t) = 0, 1$ which may be viewed as bosonic Ising-like variables. When generalized to higher dimensions unpleasant minus-signs arise which may cause problems in numerical simulations. Still, Duncan [3] could simulate a model of staggered fermions in $2 + 1$ dimensions. Later Montvay [4] refined the method and applied it to Wilson fermions in $3 + 1$ dimensions. Here I present a new construction which eliminates several constraints present in the configurations of the previous approaches. As before a nonlocal sign factor arises for the Boltzmann weight of each configuration reflecting the Fermi statistics of the original theory. Hence, the bosonic theory of occupation numbers is not fully local. However, again one may include this factor in the measured observables and view the system without the sign factor as a local bosonized theory. The resulting theory corresponds to a quantum spin system. Of course, also the sign factor may fluctuate but, as opposed to the usual fermion determinant, the fluctuations are restricted to $\pm 1$. Still, for some models this may lead to a minus-sign problem of large cancellations between configurations with positive and negative Boltzmann weights. In previous approaches to the problem the system of occupation numbers was updated using standard local Metropolis or heat bath algorithms. These algorithms are known to suffer from critical slowing down. Recently, Evertz, Lana and Marcu [5] have developed cluster algorithms for vertex models, which can also be applied to quantum spin systems. Unlike the usual Swendsen-Wang-Wolff clusters [6] the Evertz-Lana-Marcu clusters form closed loops. Since our fermion system corresponds to a quantum spin system a cluster algorithm can be applied also here.

To be specific I restrict myself to a simple model which, however, shows the characteristic features of more complicated (and physically much more interesting) fermionic systems. It is straightforward (although in some cases perhaps tedious) to apply the same ideas to more general fermionic models. I consider fermions living on the sites of a spatially 2-dimensional $L \times L$ lattice with even $L$ and with
periodic boundary conditions. The characteristic difficulties of fermion updating arise because the operators $c_x^+$ and $c_x$, which create and annihilate fermions at the lattice site $x = (x_1, x_2) \in \mathbb{Z}^2$, anticommute

$$\{c_x^+, c_y^+\} = 0, \quad \{c_x, c_y\} = 0, \quad \{c_x^+, c_y\} = \delta_{xy}. \quad (1)$$

The difficulties are due to Fermi statistics, not due to spin. For simplicity I therefore consider fermions without spin and with a Hamilton operator

$$H = \sum_{x,i} (c_x^+ c_x + c_{x+i}^+ c_{x+i} - c_x c_{x+i} - c_{x+i}^+ c_x), \quad (2)$$

where $\hat{i}$ is the unit vector in $i$-direction. The model is trivial and can be solved in momentum space by introducing $c_p^+ = \frac{1}{2} \sum_x \exp(ipx) c_x^+$, $c_p = \frac{1}{2} \sum_x \exp(-ipx) c_x$, which implies $H = \sum_p \hat{p}^2 c_p^+ c_p$ with $\hat{p}_i = 2 \sin(p_i/2)$. For example, in the grand canonical ensemble the expectation value of the occupation number $n_x = c_x^+ c_x$ of a site $x$ is given by

$$\langle n_x \rangle = \frac{1}{Z} \text{Tr}[n_x \exp(-\beta(H - \mu N))] = \frac{1}{L^2} \sum_p \frac{1}{1 + \exp(\beta(\hat{p}^2 - \mu))}, \quad (3)$$

where $\beta$ is the inverse temperature, $\mu$ is the chemical potential and $N = \sum_x n_x$ is the fermion number operator. Let us try to obtain the same result from a numerical simulation.

To write the partition function $Z$ as a path integral we first label the lattice sites $x = (x_1, x_2)$ for $x_i \in \{0, 1, ..., L - 1\}$ by $l \in \{1, 2, ..., L^2\}$ in some arbitrary order. A convenient choice for numerical applications is e.g. $l = 1 + x_1 + x_2 L$. Following Jordan and Wigner \[1\] the fermion creation and annihilation operators are represented as

$$c_x^+ = (-1)^{x_1 + x_2} \sigma^3_x \sigma^3_{x+1} \sigma_{l-1}^+, \quad c_x = (-1)^{x_1 + x_2} \sigma^3_x \sigma^3_{x+1} \sigma_{l-1}^-,$$ \quad (4)

where $\sigma^i_l$ are Pauli matrices associated with the lattice point labeled with $l$ and $\sigma_{i}^\pm = \frac{1}{2}(\sigma_{i}^1 \pm i \sigma_{i}^2)$. The different signs for $x_1 + x_2$ even and odd lattice points are not really necessary but they absorb an inconvenient minus-sign in some expressions below. I decompose the Hamiltonian into four pieces $H = H_1 + H_2 + H_3 + H_4$

$$H_1 = \sum_{x=(2m,n)} h_{x,1}, \quad H_2 = \sum_{x=(m,2n)} h_{x,2}, \quad H_3 = \sum_{x=(2m+1,n)} h_{x,1}, \quad H_4 = \sum_{x=(m,2n+1)} h_{x,2},$$ \quad (5)

where $h_{x,i} = c_x^+ c_x + c_{x+i}^+ c_{x+i} - c_x c_{x+i} - c_{x+i}^+ c_x$. The individual contributions to a given $H_j$ commute with each other, but two different $H_j$ do not commute. Using the Suzuki-Trotter formula one writes for the grand canonical partition function

$$Z = \text{Tr} \exp(-\beta(H - \mu N)) = \lim_{M \to \infty} \text{Tr}[\exp(-\epsilon \beta(H_1 - \frac{\mu}{4} N)) \times \exp(-\epsilon \beta(H_2 - \frac{\mu}{4} N)) \exp(-\epsilon \beta(H_3 - \frac{\mu}{4} N)) \exp(-\epsilon \beta(H_4 - \frac{\mu}{4} N))], \quad (6)$$
The Boltzmann factor takes the form one that occurs in path integral representations of quantum spin systems [7].

\[
\exp(-\epsilon\beta(h_{x,i} - \frac{\mu}{4} n_{x} - \frac{\mu}{4} n_{x+i})) = \exp(-\epsilon\beta(1 - \frac{\mu}{4}))
\]

\[
\times \begin{pmatrix}
\exp(\epsilon\beta(1 - \frac{\mu}{4})) & 0 & 0 & 0 \\
0 & \cosh(\epsilon\beta) & \sinh(\epsilon\beta) & \Sigma \\
0 & \sinh(\epsilon\beta) & \cosh(\epsilon\beta) & 0 \\
0 & 0 & 0 & \exp(-\epsilon\beta(1 - \frac{\mu}{4}))
\end{pmatrix},
\]

(7)

where the \(4 \times 4\) matrix is in the Fock space basis \(|00\rangle, |01\rangle, |10\rangle, |11\rangle\) of the sites \(x\) and \(x + \hat{i}\). \(\mathbb{1}\) is the identity and \(\Sigma = \sigma_{i+1}^{3} \sigma_{i+2}^{3} \ldots \sigma_{m-1}^{3}\) is a string of Pauli matrices running over consecutive labels between \(l\) and \(m\), where \(l\) labels \(x\) and \(m\) labels \(x + \hat{i}\). The operators \(\mathbb{1}\) and \(\Sigma\) act on the remaining occupation numbers and are diagonal in our basis. The partition function turns into a path integral over occupation numbers \(n(x,t) = 0,1\) (\(t\) labels the time slice) with periodic boundary conditions in the euclidean time direction

\[
Z = \prod_{x,t} \sum_{n(x,t) = 0,1} \exp(-S[n]) \text{Sign}[n].
\]

(8)

The Boltzmann factor takes the form

\[
\exp(-S[n]) = \prod_{x=(2m,n), t=4p} \exp(-s[n(x,t), n(x + \hat{1}, t), n(x, t+1), n(x + \hat{1}, t+1)])
\]

\[
\times \prod_{x=(m,2n), t=4p+1} \exp(-s[n(x,t), n(x + \hat{2}, t), n(x, t+1), n(x + \hat{2}, t+1)])
\]

\[
\times \prod_{x=(2m+1,n), t=4p+2} \exp(-s[n(x,t), n(x + \hat{1}, t), n(x, t+1), n(x + \hat{1}, t+1)])
\]

\[
\times \prod_{x=(m,2n+1), t=4p+3} \exp(-s[n(x,t), n(x + \hat{2}, t), n(x, t+1), n(x + \hat{2}, t+1)]),
\]

(9)

with \(s[0, 0, 0, 0] = 0, s[1, 1, 1, 1] = 2\epsilon\beta(1 - \frac{\mu}{4})\), \(s[0, 1, 0, 1] = s[1, 0, 1, 0] = \epsilon\beta(1 - \frac{\mu}{4}) - \ln \cosh(\epsilon\beta)\), \(s[0, 1, 1, 0] = s[1, 0, 0, 1] = \epsilon\beta(1 - \frac{\mu}{4}) - \ln \sinh(\epsilon\beta)\). All other action values are infinite. Note that the occupation numbers \(n(x,t) = 0,1\) are bosonic variables interacting with each other via the time-like plaquette couplings \(s[n(x,t), n(x + \hat{i}, t), n(x, t+1), n(x + \hat{i}, t+1)]\). This structure is identical with the one that occurs in path integral representations of quantum spin systems [\footnote{eq.}].

In addition to the Boltzmann factor each configuration is weighted by a sign factor which arises from the strings of Pauli matrices of eq.\([\footnote{eq.}]\). Just as the Boltzmann
factor \( \exp(-S[n]) \) the sign factor \( \text{Sign}[n] \) is a product of terms \( \text{sign}[n(x, t), n(x + \hat{i}, t), n(x, t + 1), n(x + \hat{i}, t + 1)] \) associated with each plaquette interaction. One has \( \text{sign}[0, 0, 0, 0] = \text{sign}[1, 1, 1, 1] = \text{sign}[0, 1, 0, 1] = \text{sign}[1, 0, 1, 0] = 1 \). A nontrivial sign \( \pm 1 \) may arise only for plaquette interactions of type \([0, 1, 1, 0]\) and \([1, 0, 0, 1]\).

To compute the sign factors it is convenient to order the \( h_{x,i} \) of each \( H_j \) in some (again arbitrary) way. The factor \( \text{sign}[n(x, t), n(x + \hat{i}, t), n(x, t + 1), n(x + \hat{i}, t + 1)] \) is the product of eigenvalues \( \pm 1 \) of \( \sigma^3_p \) for the sites with label \( p \) between \( l \) and \( m \), i.e. \( l + 1 \leq p \leq m - 1 \). Here \( l \) labels the point \( x \) and \( m \) labels the point \( x + \hat{i} \). If the \( h_{y,i} \) to which the point with label \( p \) belongs is ordered before \( h_{x,i} \) its \( 4 \times 4 \) matrix of eq.(8) has already acted on the site labeled by \( p \) and we must take its occupation number at time \( t + 1 \). If, on the other hand, \( h_{y,i} \) is ordered after \( h_{x,i} \) it has not yet acted on this site and we must take the occupation number at the earlier time \( t \). Note that an occupied site gives a factor 1 while an empty site gives a factor \(-1\). Because the individual \( h_{x,i} \) of a given \( H_j \) commute with each other their order does not influence the final result. Moreover, it turns out that the total sign factor \( \text{Sign}[n] \) is independent of the chosen ordering of lattice sites, although the contributions from individual plaquettes are in general order-dependent. Hence, any reference to the arbitrary order in the Jordan-Wigner representation has disappeared from the final expression. This is a very pleasant surprise. The sign factor is nonlocal, but it can be computed with an effort proportional to the lattice size if a convenient ordering is chosen. More is not needed because the factor is not used in the updating process. Since it cannot be interpreted as a probability it is included in the measured observables. The system without the sign factor is bosonic and interacts locally. In fact, it corresponds to a quantum spin system with Hamiltonian

\[
H = \sum_{x,i} \left( \frac{1}{2} \sigma^1_{x,i} \sigma^1_{x + \hat{i},i} + \frac{1}{2} \sigma^2_{x,i} \sigma^2_{x + \hat{i},i} + \sigma^3_{x,i} \sigma^3_{x + \hat{i},i} \right) + \left( 2 - \frac{\eta}{2} \right) \sum_x \sigma^3_x,
\]

which may be viewed as a bosonized version of the original fermionic model. This type of bosonization up to a nonlocal sign works in any dimension. In ref.[8] Ambjørn and Semenoff proceeded in the opposite direction. They fermionized a quantum spin system without the extra sign factor and they arrived at \( 2 + 1 \)-dimensional QED with a Chern-Simons term. Lüscher also used a Chern-Simons term in a general construction of bosonization in \( 2 + 1 \) dimensions both in the continuum and on the lattice [9].

The cluster algorithm of Evertz, Lana and Marcu [5], which was originally constructed for vertex models, works very well also for quantum spin systems [10]. Here I describe a variant of the algorithm suitable for updating the fermionic model. The algorithm constructs closed loops which are then flipped, i.e. the occupation numbers of points on the loop are changed from 0 to 1 and vice versa. To start a loop one first selects a lattice point \((x, t)\) at random. The occupation number \( n(x, t) \) participates in two plaquette interactions, one at euclidean times before and one at euclidean times after \( t \). For \( n(x, t) = 1 \) we consider the interaction at the later and for \( n(x, t) = 0 \) we consider the interaction at the earlier time. The corresponding plaquette configuration is characterized by the occupation numbers of four lattice points. One of these points will be the next point on the loop. For configurations \([0, 0, 0, 0]\) or \([1, 1, 1, 1]\) the next point is with probability \( \rho = \frac{1}{2} (1 + \exp(-\epsilon \beta)) \) the
time-like nearest neighbor of \((x, t)\), and with probability \(1 - p\) the next-to-nearest (diagonal) neighbor of \((x, t)\) on the plaquette. For configurations \([0, 1, 0, 1]\) or \([1, 0, 1, 0]\) the next point on the loop is with probability \(p/\cosh(\epsilon \beta)\) the time-like nearest neighbor, and with probability \(1 - p/\cosh(\epsilon \beta)\) the space-like nearest neighbor of \((x, t)\). Finally, for configurations \([0, 1, 1, 0]\) or \([1, 0, 0, 1]\) the next point is with probability \((1 - p)/\sinh(\epsilon \beta)\) the diagonal neighbor, and with probability \(1 - (1 - p)/\sinh(\epsilon \beta)\) the space-like nearest neighbor of \((x, t)\). Once the next point on the loop is determined the process is repeated until the loop closes. The above probabilities are arranged such that the algorithm obeys detailed balance. The part of the action proportional to \(1 - \frac{\mu}{4}\) is taken into account by a global Metropolis step. For this purpose each loop \(C\) is characterized by a winding number \(W(C)\), which counts how often the loop winds around the lattice in the euclidean time direction. The winding number is related to the total occupation number of the loop \(W(C) = \frac{1}{4M} \sum_{(x,t) \in C} (2n(x,t) - 1)\) where \(4M\) is the number of euclidean time slices. The action associates a Boltzmann factor \(\exp(-\beta (2 - \mu) W(C))\) with each loop. When the loop is flipped its winding number changes sign. In the Metropolis step the loop is flipped with probability \(p = \min(1, \exp(\beta (4 - \mu) W(C)))\).

I have applied the algorithm in a single cluster version for various values of \(\beta\) and \(\mu\) at fixed lattice spacing \(\epsilon \beta = 1/16\). For equilibration 100000 loop clusters have been updated, followed by 100000 measurements each separated by 10 loop updates. The Monte-Carlo (MC) results are compared to the exact results in table 1; both agree within error bars. Note that \(\langle n_x \rangle = \langle n_{2x} \text{Sign}[n] \rangle_b / \langle \text{Sign}[n] \rangle_b\) where \(b\) refers to the simulated bosonic ensemble. One can see that the minus-sign problem becomes more severe when the temperature is lowered or when the chemical potential is increased. However, only at \(\beta = 1, \mu = 4\) there is a real problem, because only then \(\langle \text{Sign}[n] \rangle_b\) is consistent with zero. A detailed analysis of the efficiency of the algorithm will be presented elsewhere.

The purpose of the present paper was to describe the bosonization scheme for lattice fermions, and to apply it to numerical simulations of a simple model. Of course, the idea is to apply the method to models of physical interest. In condensed matter physics one can attack the Hubbard model or other models relevant for high \(T_c\) superconductivity. In relativistic lattice field theories one may first study free Wilson or staggered fermions. The simplest nontrivial particle physics application is perhaps to the purely fermionic Gross-Neveu model. In general, however, the fermions are coupled to bosonic fields as well. For example, the Yukawa coupling to a scalar field corresponds to a space-time dependent chemical potential and is easy to incorporate. In QCD one wants to study the coupling of quarks to \(SU(3)\) gauge fields, which should be possible along similar lines. In all cases the minus-sign problem might raise its ugly head once one enters a physically interesting regime. Only a detailed investigation of the various models of interest can show if this is the case or not. Work in some of these directions is in progress.

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Table 1: Results of the numerical simulations.

| β  | µ  | L  | 4M | ⟨Sign[n]⟩_b | ⟨nx⟩_MC | ⟨nx⟩_exact |
|----|----|----|----|-------------|----------|------------|
| 0.25 | 0 | 8  | 16 | 0.976(1)    | 0.2798(3) | 0.27961    |
| 0.25 | 1 | 8  | 16 | 0.970(1)    | 0.3304(4) | 0.32989    |
| 0.25 | 2 | 8  | 16 | 0.964(1)    | 0.3843(5) | 0.38417    |
| 0.25 | 4 | 8  | 16 | 0.963(1)    | 0.4999(7) | 0.50000    |
| 0.50 | 0 | 8  | 16 | 0.868(2)    | 0.1555(5) | 0.15655    |
| 0.50 | 1 | 8  | 16 | 0.779(2)    | 0.223(1)  | 0.22310    |
| 0.50 | 2 | 8  | 16 | 0.686(2)    | 0.306(1)  | 0.30493    |
| 0.50 | 4 | 8  | 16 | 0.587(2)    | 0.500(3)  | 0.50000    |
| 1.00 | 0 | 8  | 64 | 0.747(2)    | 0.067(1)  | 0.06853    |
| 1.00 | 1 | 8  | 64 | 0.322(3)    | 0.137(2)  | 0.13509    |
| 1.00 | 2 | 8  | 64 | 0.052(3)    | 0.23(2)   | 0.23209    |
| 1.00 | 4 | 8  | 64 | -0.001(3)   | 0.5(1.7)  | 0.50000    |

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