Solution to new sign problems with Hamiltonian Lattice Fermions

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Review: Staggered Fermions

- Discretized version of the Dirac Hamiltonian that introduces a single fermion field component to each lattice site and interprets doubling as physical flavors.

\[
\begin{align*}
H &= t \sum_{x} \left[ i/2 \left( \delta x + \hat{\alpha}_1, y - \delta x - \hat{\alpha}_1, y \right) + i/2 \left( -1 \right) x_1 \left( \delta x + \hat{\alpha}_2, y - \delta x - \hat{\alpha}_2, y \right) \right] \\
&= t \sum_{xy} M_{xy} c^\dagger_x c_y,
\end{align*}
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- In two dimensions, given by

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\]  

(1)

- Can be written as

\[
H = t \sum_{xy} c_x^{\dagger} M_{xy} c_y,
\]  

(2)

where

\[
M_{xy} = \frac{i}{2} \left( \delta_{x+\hat{\alpha}_1,y} - \delta_{x-\hat{\alpha}_1,y} \right) + \frac{i}{2} (-1)^x \left( \delta_{x+\hat{\alpha}_2,y} - \delta_{x-\hat{\alpha}_2,y} \right).
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(3)

Particle-hole symmetry: $c_x \rightarrow \sigma_x c_x^\dagger$, $\sigma_x = (-1)^{x_1 + x_2}$
Motivation to use Hamiltonian Formalism

- No doubling in time dimension. The four zero modes at the corners of the 2d Brillouin zone can be interpreted as $N_f = 1$ (4-component) Dirac fermion.
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- There’s an issue with Hamiltonian fermions though: sign problems in some models.
- The solution? Fermion bag approach.
The Naive Method

- We begin with writing $Z = Tr \left( e^{-\beta \epsilon} \right)$ as

$$Z = Tr \left( e^{-\epsilon H} e^{-\epsilon H} e^{-\epsilon H} \ldots e^{-\epsilon H} \right)$$

(4)

where there are $N$ factors such that $N \epsilon = \beta$. 


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$$Z = \int \left[ d\bar{\psi} d\psi \right] e^{-\bar{\psi}_1 \psi_1} \left\langle -\bar{\psi}_1 | e^{-\epsilon H} | \psi_2 \right\rangle e^{-\bar{\psi}_2 \psi_2} \left\langle \bar{\psi}_2 | e^{-\epsilon H} | \psi_3 \right\rangle$$

$$e^{-\bar{\psi}_3 \psi_3} \left\langle \bar{\psi}_3 | e^{-\epsilon H} | \psi_4 \right\rangle ... e^{-\bar{\psi}_n \psi_n} \left\langle \bar{\psi}_n | e^{-\epsilon H} | \psi_1 \right\rangle$$  \hspace{1cm} (5)
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$$= \int \left[ d\phi d\bar{\psi} d\psi \right] e^{-\bar{\psi} M(\phi) \psi - S(\phi)}$$  \hspace{0.5cm} (6)
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  $$= \int \left[ d\phi \right] e^{-S[\phi]} \det M(\phi)$$ (7)
Problems with Naive Method

We have a sum of determinants. In some models this method will still work if we can find a “pairing mechanism.” Example: Even numbers of flavors can lead to squares of the determinant. But odd numbers of flavors (such as this model) typically lead to sign problems.
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- The average $\langle n \rangle \neq \frac{1}{2}$ unless $\epsilon \to 0$. 

\[ \langle n \rangle = \int d\bar{\psi} d\psi e^{-S} \bar{\psi} x \psi x \int d\bar{\psi} d\psi e^{-S} \bar{\psi} x \psi x \]
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$$\langle n_x \rangle = \frac{\int [d\bar{\psi}d\psi] e^{-S}\psi_x\bar{\psi}_x}{\int [d\bar{\psi}d\psi] e^{-S}}$$

$\langle n \rangle$ versus epsilon
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Alternative Method

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where there are $k$ insertions of $H_{\text{int}}$.

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We will see that, for a certain class of models, this expression may be written as determinants of matrices with some useful properties.
The Sign Problem in the Hamiltonian Approach

Here we focus on a specific model involving staggered fermions:

\[ H = t \sum_{x,y} c_x^\dagger M_{xy} c_y + \sum_{\langle x,y \rangle} \frac{V}{4} \left( n_x - \frac{1}{2} \right) \left( n_y - \frac{1}{2} \right) \]  \tag{9}

Similar model considered by: Gubernatis, Scalapino, Sugar, Toussaint. PRB (1985)

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At half-filling with particle-hole symmetry. Rewrite interaction using auxiliary bosonic field \( s \) (\( n_x^+ = c_x^\dagger c_x, n_x^- = 1 - n_x^+ \)):

\[ H_{\text{int}} = \frac{V}{4} \sum_{b,s_x,s_y,\langle x,y \rangle} \left( s_x n_x^{s_x} \right) \left( s_y n_y^{s_y} \right) \]  

(10)

where

\[ M_{xy}' = \left( -\frac{1}{2} \right) \left( 1 + \hat{\alpha}_{x+y} \right) \delta_{x+y,0} + \left( -\frac{1}{2} \right) \left( 1 + \hat{\alpha}_{x-y} \right) \delta_{x-y,0} , \]  

\[ M_{xy}'' = \frac{1}{4} \left( 2 \delta_{x+y,0} + 2 \delta_{x-y,0} \right) \]

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where \(M'^T = -DM'D, (D_{xy} = \sigma_x \delta_{xy})\)
The Partition Function

\[ Z = Z_0 \sum_k \sum_{[b,s]} \int [dt] \left( -\frac{V}{4} \right)^k \text{Tr} \left( e^{-(\beta-t_1)H_0} (s_{x'} n_{x'}^{s_{x'}}) (s_{y'} n_{y'}^{s_{y'}}) \right. \]

\[ \left. e^{-(t_1-t_2)H_0} (s_{x''} n_{x''}^{s_{x''}}) (s_{y''} n_{y''}^{s_{y''}}) \cdots e^{-(t_{k-1}-t_k)H_0} (s_{x(k)} n_{x(k)}^{s_{x(k)}}) (s_{y(k)} n_{y(k)}^{s_{y(k)}}) e^{-t_k H_0} \right) \]

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The G-Matrix Elements

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$$G = \begin{pmatrix}
d_{11}[s] & a_{12} & \cdots & a_{13} & a_{14} \\
-a_{12} & d_{22}[s] & \cdots & a_{23} & a_{24} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
a_{13} & a_{23} & \cdots & d_{33}[s] & a_{34} \\
a_{14} & a_{24} & \cdots & -a_{34} & d_{44}[s]
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    a_{14} & a_{24} & \vdots & -a_{34} & d_{44}[s]
\end{pmatrix} \quad (15)$$

- The following identities hold: $a_{yx} = -\sigma_x a_{xy} \sigma_y$ and $d_{xx}[s] = -\frac{s_x}{2}$.
The Sign Problem

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- In fact, in generating 10,000 such determinants randomly, we find a severe sign problem:

**Figure:** 10,000 determinants: 5004 were positive and 4996 were negative.
In our model each diagonal element can be treated as a fermion bag dependent on $[s]$. Since dependence on auxiliary bosonic field $[s]$ is freely fluctuating, we can integrate it out.
The Fermion Bag Technique

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- Thus, consider the \([s]\) sum:

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\sum_{[s]} \text{Det} (G[b, s, t])
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- We may write this determinant in Grassman integral form:

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\sum_{[s]} \int [d\bar{\psi} d\psi] \ e^{-\bar{\psi}((D_0[s]) + A([b, t]))\psi}
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(17)

- We first sum up the diagonal portion.
The Diagonal Sum

- We note that for the diagonal part:

\[
\sum_{[s]} e^{-\bar{\psi}D_0([s])\psi} = \prod_q \sum_{s_q=1,-1} \left(1 + \frac{s_q}{2} \bar{\psi}_q \psi_q\right)
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Which is simply:

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Thus our partition function is now given by:

\[
Z = \sum_{[b]} \int [dt] (-V)^k \text{Det} (A([b, t]))
\]  

(20)
Pictorial Proof

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\end{array}
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\[
\begin{array}{cc}
1 & 2 \\
2 & 1 \\
\end{array}
\]

In our sum of the $D_0 + A$ determinants, for every term of the form

\[
\begin{array}{c}
\ldots \\
\begin{array}{c}
1 \\
2 \\
\end{array} \\
\begin{array}{c}
i \\
\end{array} \\
\begin{array}{c}
s_t = 1 \\
\end{array} \\
\ldots \\
\end{array}
\]
Pictorial Proof

- Alternatively, we can see how this works using the pictorial representation of determinants. For example, a $2 \times 2$ determinant can be represented as:

\[
\begin{bmatrix}
1 & 2 \\
2 & 1 \\
\end{bmatrix}
\]

- In our sum of the $D_0 + A$ determinants, for every term of the form

\[
\begin{bmatrix}
\cdots & i \\
\cdots & s_i = 1 \\
\end{bmatrix}
\]

We have one with the form...
Pictorial Proof

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\end{pmatrix}
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\[
= 1 \quad + \quad 1
\]

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\[
\begin{pmatrix}
\cdots & i \\
\cdot & \cdot \\
\cdot & \cdot
\end{pmatrix}
\]

\[
s_i = 1
\]

We have one with the form

\[
\begin{pmatrix}
\cdots & i \\
\cdot & \cdot \\
\cdot & \cdot
\end{pmatrix}
\]

\[
s_i = -1
\]
But are the determinants positive?

- $A([t])$ satisfies the relation $A^T = -\tilde{D}A\tilde{D}$, \( (\tilde{D}_{xy} = \sigma_x \delta_{xy}) \) so:

\[
\left( A\tilde{D} \right)^T = -A\tilde{D} \quad (21)
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- But \( \text{Det} \left( \tilde{D} \right) \) is \( (-1)^k \), since there are \( k \) even sites and \( k \) odd sites. Thus:

\[
(-1)^k \text{Det} \left( A([b, t]) \right) = \text{Det} \left( A\tilde{D} \right) \geq 0
\]  
(22)
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- But $\det(\tilde{D})$ is $(-1)^k$, since there are $k$ even sites and $k$ odd sites. Thus:

$$(-1)^k \det(A([b, t])) = \det\left( A\tilde{D} \right) \geq 0 \quad (22)$$

- And we have:

$$Z = \sum_{[b]} \int [dt] (V)^k \det\left( A([b, t]) \tilde{D} \right) \quad (23)$$
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- And we have:

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  Z = \sum_{[b]} \int [dt] (V)^k \text{Det} (A([b, t]) \tilde{D})
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  \[(23)\]

- We have solved the sign problem. (For repulsive model!)
Some Example Determinants

- 100 such determinants, randomly selected. All were confirmed to be positive.
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- Note that the probability of positive weight configurations is exponentially smaller, because the -\log{det} value is larger.
Conclusions and Future Work

- Even with particle-hole symmetry, some models still have sign problems. However, we have solved a class of them.
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- Or we can add a staggered mass term that puts particles on the even sublattice and holes on the odd sublattice.
- Possible to study new quantum critical behavior.