Solution to new sign problems with Hamiltonian Lattice Fermions

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Review: Staggered Fermions

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- In two dimensions, given by

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H = t \sum_x \left[ \frac{i}{2} \left( c_x^\dagger c_{x+\hat{\alpha}_1} - c_x^\dagger c_{x-\hat{\alpha}_1} \right) + \frac{i}{2} (-1)^{x_1} \left( c_x^\dagger c_{x+\hat{\alpha}_2} - c_x^\dagger c_{x-\hat{\alpha}_2} \right) \right].
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- Can be written as

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where

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- 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 $Z = \text{Tr} \left( e^{-\beta \epsilon} \right)$ as

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

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

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

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$$= \int \left[ d\phi d\bar{\psi} d\psi \right] e^{-\bar{\psi} M(\phi) \psi - S(\phi)}$$
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$$= \int [d \phi] e^{-S[\phi]} \det M (\phi)$$
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.

$$\langle n \rangle \neq \frac{1}{2}$$ unless $$\epsilon \to 0.$$
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Figure:
$\langle n \rangle$ approaches $\frac{1}{2}$ as $\epsilon \to 0$. 
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$$\langle n_x \rangle = \frac{\int \left[ d\bar{\psi}d\psi \right] e^{-S}\psi_x\bar{\psi}_x}{\int \left[ d\bar{\psi}d\psi \right] e^{-S}}$$

![Graph showing $\langle n \rangle$ versus epsilon]
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Alternative Method

- Particle-hole symmetry is recovered in a continuous time formulation. (Can this help us?)
- We note that $H = H_0 + H_{\text{int}}$. Then we expand and get the following:
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$$Z = \sum_k \int [dt] (-1)^k \text{Tr} \left( e^{-(\beta-t)H_0} H_{\text{int}} e^{-(t_1-t_2)H_0} H_{\text{int}} \ldots \right) ,$$  \hspace{1cm} (8)

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

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


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)

\[ V \geq 2t: \text{Chandrasekharan, Cox, Holland, Wiese. Nucl. Phys. (1999).} \]
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At half-filling with particle-hole symmetry. Rewrite interaction using auxiliary bosonic field \( s \) (\( n_x^+ = c_x^\dagger c_x, n_x^- = 1 - n_x^+ \)):

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

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Particle-hole symmetry is preserved. Making unitary transformations:

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H = t \sum_{x,y} d_x^{\dagger} M'_{xy} d_y + \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) \tag{11}
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where \( M'^T = -DM'D, (D_{xy} = \sigma_x \delta_{xy}) \)
The Partition Function

\[
Z = Z_0 \sum_k \sum_{[b,s]} \int [dt] \left( -\frac{V}{4} \right)^k \text{Tr} \left( e^{-\left(\beta - t_1\right)H_0} \left( s_{x'} n_{x'}^{s_{x'}} \right) \left( s_{y'} n_{y'}^{s_{y'}} \right) \right) e^{-\left( t_1 - t_2 \right)H_0} \left( s_{x''} n_{x''}^{s_{x''}} \right) \left( s_{y''} n_{y''}^{s_{y''}} \right) \cdots e^{-\left( t_{k-1} - t_k \right)H_0} \left( s_{x^{(k)}} n_{x^{(k)}}^{s_{x^{(k)}}} \right) \left( s_{y^{(k)}} n_{y^{(k)}}^{s_{y^{(k)}}} \right) e^{-t_k H_0} \right)
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e^{-(t_1 - t_2)H_0 (s_{x''} n_{x''}^{s''}) (s_{y''} n_{y''}^{s''})} \cdots e^{-(t_{k-1} - t_k)H_0 (s_{x(k)} n_{x(k)}^{s(x(k))}) (s_{y(k)} n_{y(k)}^{s(y(k))})} e^{-t_k H_0}
\]
The G-Matrix Elements

This trace can be evaluated exactly in terms of the determinant of a $2k \times 2k$ matrix, $G([b, s, t])$. 

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

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The following identities hold:

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Huffman and Chandrasekharan (Duke)
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The Sign Problem

- However, no guarantee that these determinants will be positive. Under particle-hole symmetry, \([s] \rightarrow [-s]\), so not symmetric for fixed \(s\).

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.
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**Figure:** 10,000 determinants: 5004 were positive and 4996 were negative.
The Fermion Bag Technique

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.
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- We may write this determinant in Grassman integral form:

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\sum_{[s]} \int \left[ d\bar{\psi} d\psi \right] 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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- Thus our partition function is now given by:

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

(20)
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:
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\[
\begin{array}{c}
1 \\
\circlearrowleft \\
2 \\
\circlearrowleft \\
\end{array}
+ 
\begin{array}{c}
1 \\
\circlearrowright \\
2 \\
\circlearrowright \\
\end{array}
\]
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\[
\begin{array}{cc}
1 & 2 \\
\end{array}
\begin{array}{cc}
+ & 1 & 2
\end{array}
\]

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

\[
\begin{array}{c}
\circlearrowleft \\
\ldots \\
\circlearrowleft \\
\circlearrowleft \\
\ldots \\
\end{array}
\]

\[
i \circlearrowleft \\
_{s_i = 1}
\]

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

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

\[
\begin{array}{cccc}
& & & \\
& \circ & & \circ \\
\end{array} \quad \ldots \quad \begin{array}{cccc}
& & & \\
& \circ & & \circ \\
\end{array} \quad \ldots
\]

We have one with the form
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:

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

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

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

  We have one with the form

  \[
  \begin{array}{cc}
  \cdots & i \\
  s_i = -1 & \cdots \\
  \end{array}
  \]
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:

\[
(\tilde{A}\tilde{D})^T = -\tilde{A}\tilde{D}
\]  

(21)
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  $$\left( A\tilde{D} \right)^T = -A\tilde{D}$$  \hspace{1cm} (21)

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

- And we have:

  \[
  Z = \sum_{[b]} \int [dt] (V)^k \text{Det}(A([b, t]) \tilde{D})
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  \[
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  \] (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 $-\log\text{det}$ 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.