The Fermion Bag Approach

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In collaboration with Shailesh Chandrasekharan
- Motivation
- Monte Carlo simulation
- Sign problem
  - Fermion sign problem
  - Solutions to the sign problem
- Fermion bag approach
  - Massless Thirring model
- Conclusion
QCD phase diagram

First principles simulation at nonzero density is still unavailable
Phase diagram of High $T_c$ Material

The first principle within “Good model” calculation is still missing
Reason?

Sign problem!
Monte Carlo simulation

- Quantum fluctuation is important
- Strong interactions
- Many degree of freedom
- Analytic first principle calculations are difficult

Monte Carlo method is the only known first principle approach to solve strongly correlated problems
Monte Carlo simulation

Problems of interest are converted to a classical statistical mechanics problem

$$Z = \sum_{[s]} W([s])$$

Where $W([s]) > 0$ is the Boltzmann weight of the configuration $[s]$

The Monte Carlo method allows one to generate important configurations $[s]$, thus compute expectation values efficiently
But for quantum partition functions this is not always possible!

\[
Z = \text{Tr} \left\{ \exp\left( -\frac{H}{T} \right) \right\}
\]

*Where \( H \) is a Hermitian operator*

\[
Z = \sum_{[s_1, s_2, \ldots, s_{M-1}]} \langle s_0 | e^{-\varepsilon H} | s_{M-1} \rangle \langle s_{M-1} | e^{-\varepsilon H} | s_{M-2} \rangle \ldots \langle s_2 | e^{-\varepsilon H} | s_1 \rangle \langle s_1 | e^{-\varepsilon H} | s_0 \rangle
\]

Although \( Z \) is guaranteed to be real and positive, each term in the sum can in general be complex!

Let us define

\[
\Omega(s_0, s_1, \ldots, s_{M-2}, s_{M-1}) = \langle s_0 | e^{-\varepsilon H} | s_{M-1} \rangle \langle s_{M-1} | e^{-\varepsilon H} | s_{M-2} \rangle \ldots \langle s_2 | e^{-\varepsilon H} | s_1 \rangle \langle s_1 | e^{-\varepsilon H} | s_0 \rangle
\]

clearly

\[
\Omega(s_0, s_1, \ldots, s_{M-2}, s_{M-1}) = (\Omega(s_0, s_{M-1}, \ldots, s_2, s_1))^* 
\]
So if we define

\[ W([s]) = |\text{Real}\{\Omega(s_0, s_1, ..., s_{M-1}, s_M)\}| \]

\[ \text{Sign}([s]) = \text{Sign}(\text{Real}\{\Omega(s_0, s_1, ..., s_{M-1}, s_M)\}) \]

We can only guarantee that we can write

\[ Z = \sum_{[s]} \text{Sign}([s])W([s]) \]

If the partition function has the above form with configurations [s] such that \( \text{Sign}[s] = -1 \), we say this particular “representation” of \( Z \) has a sign problem.
Can we find representation to make sign always to be 1?

Solution to sign problem
Need fresh new ideas to solve sign problem
The sign problem

Suppose we wish to measure an observable \( \langle O \rangle \)

\[
\langle O \rangle = \frac{1}{Z} \sum_{[s]} O([s]) \text{Sign}([s]) W([s])
\]

\[
Z = \sum_{[s]} \text{Sign}([s]) W([s])
\]

The brute force method produces \([s]\) according to the distribution

\[
P([s]) = \frac{W([s])}{\sum_{[s]} W([s])}
\]

In a sense we have defined a new “classical” partition function for \([s]\)

\[
Z_c = \sum_{[s]} W([s]) \neq Z
\]
We can see that
\[
\langle O \rangle = \frac{Z_c}{Z} \frac{1}{Z_c} \sum_{[s]} O([s]) \text{Sign}([s]) W([s])
\]

We can define
\[
\langle \text{Sign} \rangle_c = \frac{\sum_{[s]} \text{Sign}([s]) W([s])}{\sum_{[s]} W([s])} = \frac{Z}{Z_c}
\]

Thus we get
\[
\langle O \rangle = \frac{\langle O \text{ Sign} \rangle_c}{\langle \text{Sign} \rangle_c}
\]

Generically since \(Z\) and \(Z_c\) are partition functions in the thermodynamic limit we expect
\[
\langle \text{Sign} \rangle_c = \frac{Z}{Z_c} = \exp \left( -\Delta f \frac{V}{T} \right)
\]

Usually \(<\text{Sign}> is exponentially small at large \(V\) and low \(T\)!
Thus, the signal for \(<O> will be exponentially noisy.
A fresh look at the fermion path integral
What does the Grassmann path integral (on the lattice) mean?

\[ Z = \text{Tr}(e^{-H/T}) = \int [d\bar{\psi} \, d\psi] \, e^{-S(\psi, \bar{\psi})} \]

There are statements in the literature which say

“... there is no way to represent Grassmann variables on a computer so we integrate them away! ...”

But we will argue that Grassmann variables help enumerate “fermionic world-line” configurations
Here $\psi$ and $\bar{\psi}$ are Grassmann valued fields on a Hypercubic lattice

Grassmann integration

\[ \int d\psi = 0 \quad \int d\psi \, \psi = 1 \quad \psi^2 = 0 \quad \psi_1 \psi_2 = -\psi_2 \psi_1 \]

Example: Free staggered fermion

\[ S(\psi, \bar{\psi}) = - \sum_{<ij>} \{ \eta_{ij} \bar{\psi}_i \psi_j + \eta_{ji} \bar{\psi}_j \psi_i \} - m \sum_i \bar{\psi}_i \psi_i \]

What does the partition function of this theory mean?
The partition function is made of products of terms on each bond. Each of this term can be one of the following:

\[ e^{\eta_{ij} \bar{\psi}_i \psi_j} = 1 + \eta_{ij} \bar{\psi}_i \psi_j \]

\[ e^{m \bar{\psi}_i \psi_i} = 1 + m \bar{\psi}_i \psi_i \]

Grassmann nature:
- Each site can have one incoming and one outgoing line
- There are sign factors that come from Grassmann ordering.

Grassmann variables help enumerate “world-lines” which are **self avoiding** loops!
Fermion World-line configuration from Grassmann Variable

Monomers = mass terms

Fermion loop
Thus, the fermionic partition function can be written as

\[ Z = \sum_{C \in \text{fermion loops}} \text{Sign}([C]) W([C]) \]

The sign function depends on the loop and the model.
- Signs factors come from local phases.
- Every fermion loop has a negative sign.

Can we solve fermion sign problems?

Research over the past decade shows that the fermion sign problem can be solved in many ways!

*Fermion determinant approach (oldest), meron cluster, fermion bag approach*
Solutions to the fermion sign problem

• Resummation over a class of world-line configurations

The fermion determinant approach is clearly one well known solution!

\[ Z = \int [d\psi \, d\bar{\psi}] \, e^{\bar{\psi}M\psi} = \sum_{[C]} \text{Sign} ([C])W([C]) = \text{Det} M \]

Can be positive! (?)

We will use this result later in Fermion bag approach
What about interacting fermions?
Massless Thirring Model

\[ S(\psi, \bar{\psi}) = - \sum_{\langle ij \rangle} \{ \eta_{ij} (\bar{\psi}_i \psi_j - \bar{\psi}_j \psi_i) + U \bar{\psi}_i \psi_i \bar{\psi}_j \psi_j \} \]

The theory contains a \( U_c (1) \times U_f (1) \) symmetry

\( U_c (1) \) is a “chiral symmetry”

\[ \psi_x \rightarrow e^{i(-1)^x \theta} \psi_x, \bar{\psi}_x \rightarrow \bar{\psi}_x e^{i(-1)^x \theta} \]

By a proper choice of the \( \eta_{ij} \) we can get massless Dirac fermions.

In the lattice QCD literature these are called staggered fermions.
A similar quantum critical point is of interest in the physics of Graphene
Conventional Approach

\[ S(\psi, \bar{\psi}) = - \sum_{\langle ij \rangle} \{ \eta_{ij} (\bar{\psi}_i \psi_j - \bar{\psi}_j \psi_i) + U \bar{\psi}_i \psi_i \bar{\psi}_j \psi_j \} \]

Using the Hubbard-Stratanovich transformation

\[ e^{U \bar{\psi}_i \psi_i \bar{\psi}_j \psi_j} = \int \frac{d\phi}{2\pi} e^{\sqrt{U} \left[ \eta_{ij} (e^{i\phi} \bar{\psi}_i \psi_j - e^{-i\phi} \bar{\psi}_j \psi_i) \right]} \]

We can then write

\[ S(\psi, \bar{\psi}, \phi) = - \sum_{\langle ij \rangle} \{ \eta_{ij} (1 + \sqrt{U} e^{i\phi_{ij}}) \bar{\psi}_i \psi_j - \eta_{ij} (1 + \sqrt{U} e^{-i\phi_{ij}}) \bar{\psi}_j \psi_i \} \]
Thus we have written the action as fermion bilinear

\[ S(\psi, \bar{\psi}, \phi) = -\bar{\psi}_i M([\phi])_{ij} \psi_j \]

So we can now write

\[ Z = \int d\phi \int [d\bar{\psi} \, d\psi] \, e^{-\bar{\psi}_i M([\phi])_{ij} \psi_j} = \int d\phi \, \text{Det}(M([\phi])) \]

Positive determinant: sign problem solved!

But...
$$S(\psi, \bar{\psi}, \phi) = -\sum_{\langle ij \rangle} \{ \eta_{ij} (1 + \sqrt{U} e^{i\phi_{ij}}) \bar{\psi}_i \psi_j - \eta_{ij} (1 + \sqrt{U} e^{-i\phi_{ij}}) \bar{\psi}_j \psi_i \}$$

When $U \to U_c \sim 1$, fluctuation due to the auxiliary field could produce zero modes

= zero weight
(odd number of sites)
But at the cost of the following:

- For large $U$, the matrix $M$ has a large number of small eigenvalues and zero modes.

- The problem has become completely non-local! ($M$ is $V \times V$ matrix)

- Monte Carlo Algorithms become inefficient!

**Massless limit is usually difficult (like QCD)!**
“... every theoretical physicist who is any good knows six or seven different theoretical representations for exactly the same physics.”

—R. P. Feynman
Fermion bag approach I

Instead of the Hubbard Stratanovich, consider writing

\[ Z = \int [d\psi \ d\bar{\psi}] \ e^{-S_0(\psi,\bar{\psi})} \prod_{<ij>} (1 + U\bar{\psi}_i\psi_j\bar{\psi}_j\psi_j) \]

free fermions

\[ Z = \sum_{[b]} \left( \prod_{ij} U^{bij} \right) \left\{ \sum_{\text{free fermions}} \text{Sign}([C, b])W([C, b]) \right\} \]

Here free fermions hop on a lattice not touched by \( b=1 \) bonds.

\[ Z = \sum_{[b]} \left( \prod_{ij} U^{bij} \right) \text{Det}(Q([b])) \]

Positive defined

\( = \text{Det}(Q([b])) \)

S. C. PRD 82:025007, 2010
$e^{U\bar{\psi}_i\psi_i\bar{\psi}_j\psi_j} = 1 + U\bar{\psi}_i\psi_i\bar{\psi}_j\psi_j = \begin{array}{cc} \bullet & \bullet \\ i & j \end{array} \begin{array}{cc} \bullet & \bullet \\ i & j \end{array}$

\[ \text{Det}(Q([b])) = \prod_i \text{Det}(Q([B_i])) \]

fermions are free inside certain regions “Bag Model”

At large $U$ the “bags” are small, so fermions are confined in small regions.
Efficient at large $U$

The effort to compute the determinant is “optimal”
Features

- Determinantal Monte Carlo
- Ratio of the determinant = inverse of matrix element needs to be computed at each local step
- Size of the matrix is optimal at large U depends on the interaction, does not scale with volume
- Small U, size scales with the volume, and is not optimal
Fermion bag approach II

\[ Z = \int d\psi \ d\bar{\psi} \ e^{-\bar{\psi}D\psi + U\bar{\psi}_x \psi_x \bar{\psi}_{x+\alpha} \psi_{x+\alpha}} \]

\[ = \int d\psi \ d\bar{\psi} \ \prod_{x,\alpha} (1 + U\bar{\psi}_x \psi_x \bar{\psi}_{x+\alpha} \psi_{x+\alpha}) \ e^{-\bar{\psi}D\psi} \]

\[ = \sum_x \sum_{N=1}^{V/2} \int d\psi \ d\bar{\psi} \ U^N \bar{\psi}_{x_1} \psi_{x_1} \bar{\psi}_{x_2} \psi_{x_2} \cdots \bar{\psi}_{x_{2N}} \psi_{x_{2N}} \ e^{-\bar{\psi}D\psi} \]

What does the partition function of this theory mean?

S. C. & A. Li
Examples of 1 bond

\[ \int d\psi \, d\bar{\psi} \, (U \bar{\psi}_1 \psi_1 \, \bar{\psi}_2 \psi_2) \, e^{-\bar{\psi} D \psi} = -S_{12} S_{21} U \]

Wick contraction

\[ S_{12} \rightarrow \text{Free fermion propagator from site 1 to site 2} \]

\[ \text{Det} \begin{pmatrix} 0 & S_{12} \\ S_{21} & 0 \end{pmatrix} = -S_{12} S_{21} \]

Massless fermion
2a translational invariant

\[ S_{12} = -S_{21} \quad \text{Anti-PBC} \]
Examples of 2 bonds

\[ \int d\psi \ d\bar{\psi} \ (U^2 \bar{\psi}_1 \psi_1 \bar{\psi}_2 \psi_2 \bar{\psi}_3 \psi_3 \bar{\psi}_4 \psi_4) \ e^{-\bar{\psi}D\psi} \]

\[ = U^2(S_{12}S_{21}S_{43}S_{34} - S_{12}S_{23}S_{34}S_{41} - S_{14}S_{43}S_{32}S_{21} + S_{14}S_{41}S_{23}S_{32}) \]
\[
\text{Det} \begin{pmatrix}
0 & S_{12} & S_{14} \\
S_{21} & S_{23} & 0 \\
S_{41} & S_{43} & 0
\end{pmatrix}
\]

\[
= S_{12}S_{21}S_{43}S_{34} - S_{12}S_{23}S_{34}S_{41} - S_{14}S_{43}S_{32}S_{21} + S_{14}S_{41}S_{23}S_{32}
\]

The partition function can be rewritten as

\[
\text{Det} \left[ \begin{pmatrix} 0 & M \\ -M^T & 0 \end{pmatrix} \right]
\]

\[
Z = \sum_x \sum_{N} \left( \text{Det}M \right)^2 U^N
\]
Efficient for small number of bonds or at small $U$

$Z = \text{Det}M_0 \left( 1 + U^\# + U^2\# + \cdots + U^{\sqrt{2}^\#} \right)$

9 × 9 matrix determinant
Compared to conventional approach V × V matrix determinant
Close to $U_c$

$N \sim 7000$ for $40^3$ lattice size

$N \sim 4000$ for $30^3$ lattice size
Benchmark of the algorithm

• Determinant calculation by SuperLU, $4000 \times 4000$ matrix costs 30 secs on single core
• Generate one independent configuration on a $30^3$ volume costs 1.5 days on single core
• Measurement of chiral condensation and its susceptibility becomes straightforward
• **Massless limit is not a problem**

*Results are coming within few weeks...*
Conclusion

• Fermion bag approach offer an alternative and powerful approach to fermion lattice field theories
• Applicable in general where sign problem are solved in conventional approach
• It is also determinant Monte Carlo method where the size of the matrix is optimized by interactions
• It can be used to solve some new sign problems
• Potential applications in the studies of graphene, unitary fermion gas, nuclear effective field theory!

The potential of the method remains largely unexplored.
Backup slides
4D QED Wilson fermions

\[ Z = \int [d\phi] \text{Det} \left( D_W [\phi] \right) \]

\[ (D_W [\phi])_{x,y} = - \sum_{\alpha} \delta_{x+\alpha,y} \Gamma_+^\alpha e^{i\phi_{x,\alpha}} + \delta_{x,y+\alpha} \Gamma_-^\alpha e^{-i\phi_{y,\alpha}} + \frac{1}{\kappa} \delta_{x,y} \]

\[ \gamma_5 D_W \gamma_5 = D_W \]

\[ \kappa < \kappa_c = 0.5 \]

Eigenvalues of \( D_W \) are either real or come in complex conjugate pairs

\[ \kappa > \kappa_c \]

Negative eigenvalues

Sign problem
Fermion bag approach

Integrate U(1) gauge

\[
\int \frac{d\phi}{2\pi} \exp(\bar{\psi}_x \Gamma^\alpha + e^{i\phi} \psi_{x+\alpha} + \bar{\psi}_{x+\alpha} \Gamma^\alpha e^{-i\phi} \psi_x) = \sum_{k=0}^{4} \frac{(\bar{\psi}_x \Gamma^\alpha \psi_{x+\alpha} \bar{\psi}_{x+\alpha} \Gamma^\alpha \psi_x)^k}{(k!)^2}.
\]

\[
e^{-\bar{\psi}_\psi/\kappa} = \sum_{n=0}^{4} \left(\frac{1}{\kappa}\right)^n \frac{[-\bar{\psi}_x \psi_x]^n}{n!}.
\]

Integrate Grassmann variables using the identity

\[
\int [d\psi] [d\bar{\psi}] (\bar{\psi})_{i_1} \psi_{j_1} (\bar{\psi})_{i_2} \psi_{j_2} (\bar{\psi})_{i_3} \psi_{j_3} (\bar{\psi})_{i_4} \psi_{j_4} = \varepsilon_{i_1i_2i_3i_4} \varepsilon_{j_1j_2j_3j_4}
\]

\[
Z = \sum_{[n,k]} \prod_B (\omega_B[n,k])
\]
Type (0,0) (simple) bag
Type (4,0) (complex) bag
Type (2,0) (complex) bag
Type (2,1) bags (complex) bag
Solution to the sign problem
Model without sign problem

\[ S = - \sum_{x, \alpha} \left( \bar{\psi}_x \psi_x \bar{\psi}_x \Gamma_+^\alpha e^{i\phi_{x,\alpha}} \psi_{x+\alpha} + \bar{\psi}_{x+\alpha} \psi_{x+\alpha} \bar{\psi}_{x+\alpha} \Gamma_-^\alpha e^{-i\phi_{x,\alpha}} \psi_x \right) + \frac{1}{\kappa} \sum_x \bar{\psi}_x \psi_x \]
In QCD quarks acquire a mass through dynamics!

How?

The “MIT Bag” model provides a very intuitive way to understand it

Can this picture emerge starting from a QCD partition function?
multilevel resummations  Lüscher, Weisz  JHEP 0109:010,2001

• A Clever representations
  world-line approach : complex scalar field theory with chemical potential

• Combine resummation and clever representations
  meron cluster  S. Chandrasekharan, U. Wiese  PRL. 83 (1999) 3116-3119

“Fermion bag approach”