# Solution to Sign Problems in p-h symmetric spin-less fermion systems 

Shailesh Chandrasekharan Duke University

Collaborator: Emilie Huffman
Work supported by US Department of Energy

## Outline

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- Motivation


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Q Particle-Hole (p-h) symmetry

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- Particle-Hole ( $p-h$ ) symmetry
- Loss of p-h symmetry


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Q Can we solve sign problems in systems containing odd numbers of NR fermions OR minimally doubled $R$ fermions?

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H=-\varepsilon\left(C_{1}^{\dagger} C_{2}+C_{2}^{\dagger} C_{1}\right)
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states:

$$
-\mathrm{O}-\longleftrightarrow-\mathrm{O}-
$$



Thermal Average

$$
\left\langle C_{i}^{\dagger} C_{i}\right\rangle_{T}=\frac{1}{2}
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partition function

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Z=\operatorname{Tr}\left(\mathrm{e}^{-H / T}\right)
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\begin{gathered}
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=--2+-\infty-+-\infty
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Easy to see why $\left\langle C_{i}^{\dagger} C_{i}\right\rangle_{T}=\frac{1}{2}$

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\begin{gathered}
Z=\int[d \bar{\psi} d \psi] \mathrm{e}^{-S(\bar{\psi}, \psi)} \\
S=-\sum_{t}\left\{\sum_{i}\left(\bar{\psi}_{i, t+1}-\bar{\psi}_{i, t}\right) \psi_{i, t}+\Delta \sum_{i, j} \bar{\psi}_{i, t} M_{i j} \psi_{j, t}\right\}
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discrete time formulations preserving p-h symmetry are indeed possible.

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What is the p-h symmetry here?
p-h symmetry $\quad C_{i} \rightarrow \sigma_{i} C_{i}^{\dagger}$,

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\sigma_{i}=\left\{\begin{array}{cc}
+1 & \text { even lattice } \\
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Potential term invariant due to the fact that

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\left(n_{i}-\frac{1}{2}\right) \rightarrow-\left(n_{i}-\frac{1}{2}\right)
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\left(n_{i}-\frac{1}{2}\right)\left(n_{j}-\frac{1}{2}\right)=n_{i} n_{j}-\frac{1}{2}\left(n_{i}+n_{j}\right)+\frac{1}{4}
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Instead note that

$$
\left(n_{i}-\frac{1}{2}\right)=\frac{1}{2}\left(C_{i}^{\dagger} C_{i}-C_{i} C_{i}^{\dagger}\right)
$$

## Hence define

$$
\begin{array}{ll}
n_{i}^{+}=C_{i}^{\dagger} C_{i} & \text { particle number } \\
n_{i}^{-}=C_{i} C_{i}^{\dagger} \quad \text { hole number }
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We will see that " $s$ " acts as an auxiliary "bosonic" field. under p-h symmetry $s \rightarrow-s$

We write

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H_{0}=\sum_{i j} C_{i}^{\dagger} M_{i j} C_{j} \quad H_{\mathrm{int}}=\frac{V}{4} \sum_{b=\langle i j\rangle, s_{i}, s_{j}} s_{i} n_{i}^{s_{i}} s_{j} n_{j}^{s_{j}}
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Using standard techniques can then write

$$
Z=\sum_{k} \int\left[d t_{1} \ldots d t_{k}\right](-1)^{k} \operatorname{Tr}\left(\mathrm{e}^{-\left(\beta-t_{1}\right) H_{0}} H_{i n t} \mathrm{e}^{-\left(t_{1}-t_{2}\right) H_{0}} H_{i n t} \ldots \mathrm{e}^{-t_{k} H_{0}}\right)
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Continuous time Monte Carlo:

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\begin{gathered}
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& \text { [b,t,s] configuration }
\end{aligned}
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& \text { We insert } \quad H_{\text {int }}=\frac{V}{4} \sum_{b=\langle i j\rangle, s_{i}, s_{j}} s_{i} n_{i}^{s_{i}} s_{j} n_{j}^{s_{j}} \quad \text { into } \\
& Z=\sum_{k} \int\left[d t_{1} \ldots d t_{k}\right](-1)^{k} \operatorname{Tr}\left(\mathrm{e}^{-\left(\beta-t_{1}\right) H_{0}} H_{\text {int }} \mathrm{e}^{-\left(t_{1}-t_{2}\right) H_{0}} H_{\text {int } \left.\ldots \mathrm{e}^{-t_{k} H_{0}}\right)}\right. \\
& \text { [b,t,s] configuration } \\
& Z=Z_{0} \sum_{k} \int[d t] \sum_{[b, s]} W([b, t, s])
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$$

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$Z_{0} W([b, t, s])=\left(-\frac{V}{4}\right)^{k} \operatorname{Tr}\left(\mathrm{e}^{-\left(\beta-t_{1}\right) H_{0}} s_{i_{1}} n_{i_{1}}^{s_{i_{1}}} s_{i 2} n_{i_{2}}^{s_{12}} \mathrm{e}^{-\left(t_{1}-t_{2}\right) H_{0}} s_{i_{3}} n_{i_{3}}^{s_{i_{3}}} s_{i_{4}} n_{i_{4}}^{s_{4}} \ldots e^{-t_{k}} H_{0}\right)$

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Z_{0} W([b, t, s])=\left(-\frac{V}{4}\right)^{k} \underbrace{\operatorname{Tr}\left(\mathrm{e}^{-\left(\beta-t_{1}\right) H_{0}} s_{s_{1}} n_{11}^{s_{1}} s_{i_{2}} n_{i_{2}}^{s_{1}} \mathrm{e}^{-\left(t_{1}-t_{2}\right) H_{0}} s_{i_{3}} n_{i_{3}}^{s_{13}} s_{i_{4}} n_{i_{4}}^{s_{i_{4}}} \ldots \mathrm{e}^{-t_{k} H_{0}}\right)}_{Z_{0} \operatorname{Det}(G[b, t, s])}
$$

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$$

## Surprise: The [s] dependence is only through diagonal terms!

## The Sign Problem

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$$
\begin{aligned}
& 5028 \text {-ve } \\
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Severe Sign Problem!

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This is possible because

$$
G([b, t, s])=\underset{\text { diagonal }}{D_{0}([s])}+\underset{\text { offdiagonal }}{A([b, t])} \begin{gathered}
\text { insight from } \\
\text { fermion bag approach }
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$$

## Insight from Fermion Bag Approach

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Q In the present case each "diagonal element" can be treated as an independent fermion bag depending on [s].

- Since the dependence on the auxiliary field [ s ] is freely fluctuating, it can be completely integrated out!

Mathematically

## Mathematically

$$
\sum_{[s]} \operatorname{Det}(G[b, t, s])=\sum_{[s]} \int[d \bar{\psi} d \psi] \mathrm{e}^{-\bar{\psi}\left(D_{0}([s])+A([b, t])\right) \psi}
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Hence, $Z=Z_{0} \sum_{k} \int[d t] \sum_{[b]}(-V)^{k} \operatorname{Det}(A([b, t]))$

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\sum_{[s]} \operatorname{Det}(G[b, t, s])=\sum_{[s]} \int[d \bar{\psi} d \psi] \mathrm{e}^{-\bar{\psi}\left(D_{0}([s s)+A([b, t])) \psi\right.} \\
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Sign problem solved?? p-h symmetric!

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$\tilde{D} A$ is real

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$$

$\operatorname{Det}(\tilde{D} A)=(-1)^{k} \operatorname{Det}(A([b, t]) \geq 0$

Thus, finally

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Z=Z_{0} \sum_{k} \int[d t] \sum_{[b]} V^{k} \operatorname{Det}(\tilde{D} A([b, t]))
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Sign problem solved for $\mathrm{V}>0$ (repulsive interactions)!

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The sign problem remains unsolved for $\mathrm{V}<0$ (attractive interations)!

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- Example of solution to a "repulsive" model!
- The solution found here is yet another application of the fermion bag idea.


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