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

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Collaborator: Emilie Huffman Work supported by US Department of Energy





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- Particle-Hole (p-h) symmetry

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 - Single species of Hamiltonian staggered fermions are harder.
- Can we solve sign problems in systems containing odd numbers of NR fermions OR minimally doubled R fermions?

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Here we will show that p-h symmetry can help solve some sign problems.

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Thermal Average

 $\langle C_i^{\dagger} C_i \rangle_T = \frac{1}{2}$

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Easy to see why
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$$S = -\sum_{t} \left\{ \sum_{i} (\overline{\psi}_{i,t+1} - \overline{\psi}_{i,t}) \psi_{i,t} + \Delta \sum_{i,j} \overline{\psi}_{i,t} M_{ij} \psi_{j,t} \right\}$$

 $Z = 1 + (1 - \varepsilon \Delta)^{1/(T\Delta)} + (1 + \varepsilon \Delta)^{1/(T\Delta)} + (1 - \varepsilon \Delta)^{1/(T\Delta)} (1 + \varepsilon \Delta)^{1/(T\Delta)}$

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Since
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in the continuous time limit we do get

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discrete time formulations preserving p-h symmetry are indeed possible.

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$$H = \sum_{\langle ij \rangle} -t_{ij} \left(C_i^{\dagger} C_j + C_j^{\dagger} C_i \right) + V \left(n_i - \frac{1}{2} \right) \left(n_j - \frac{1}{2} \right)$$

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Consider spin-less fermions moving on a bi-partite lattice with nearest neighbor interactions (all real couplings),

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By choosing $t_{ij} = t$ and a honeycomb lattice this is a relativistic Gross-Neveu model with N_f = 1 four component Dirac fermions.

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What is the p-h symmetry here?

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Potential term invariant due to the fact that

$$\left(n_i-\frac{1}{2}\right) \rightarrow -\left(n_i-\frac{1}{2}\right)$$

It is tempting to expand

$$\left(n_i - \frac{1}{2}\right)\left(n_j - \frac{1}{2}\right) = n_i n_j - \frac{1}{2}(n_i + n_j) + \frac{1}{4}$$

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Instead note that

$$\left(n_i-\frac{1}{2}\right) = \frac{1}{2}\left(C_i^{\dagger}C_i-C_iC_i^{\dagger}\right)$$

Hence define

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and write

$$\left(n_{i}-\frac{1}{2}\right)\left(n_{j}-\frac{1}{2}\right) = \frac{1}{4}\sum_{s_{i},s_{j}=\pm 1}s_{i}n_{i}^{s_{i}}s_{j}n_{j}^{s_{j}}$$

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We will see that "s" acts as an auxiliary "bosonic" field.

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under p-h symmetry $s \rightarrow -s$

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Using standard techniques can then write

$$Z = \sum_{k} \int [dt_1 \dots dt_k] (-1)^k \operatorname{Tr} \left(e^{-(\beta - t_1)H_0} H_{int} e^{-(t_1 - t_2)H_0} H_{int} \dots e^{-t_k H_0} \right)$$

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Continuous time Monte Carlo:

Beard, Wiese(1996), Sandvik (1998), Prokof'ev, Svistunov (1998), Rubtsov, Savkin Lichtenstein (2005), many others in CM community

We insert
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[b,t,s] configuration

$$Z = Z_0 \sum_k \int [dt] \sum_{[b,s]} W([b, t, s])$$

$$= \frac{1}{4} \int [dt] \sum_{[b,s]} W([b, t, s])$$

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$$Z_0 W([b, t, s]) = \left(-\frac{V}{4}\right)^k \operatorname{Tr}\left(e^{-(\beta - t_1)H_0} s_{i_1} n_{i_1}^{s_{i_1}} s_{i_2} n_{i_2}^{s_{i_2}} e^{-(t_1 - t_2)H_0} s_{i_3} n_{i_3}^{s_{i_3}} s_{i_4} n_{i_4}^{s_{i_4}} \dots e^{-t_k H_0}\right)$$

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$$Q_{k} \times 2k \text{ matrix}$$

$$G_{q \ q'} = -\sigma_{i_{q}} \sigma_{i_{q'}} G_{q'q} q > q'$$

$$G_{q \ q} = -\frac{Sq}{2}$$

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

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Severe Sign Problem!



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- 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!

$$\sum_{[s]} \operatorname{Det}(G[b, t, s]) = \sum_{[s]} \int [d\overline{\psi} \ d\psi] \ e^{-\overline{\psi}(D_0([s]) + A([b, t]))} \psi$$

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A([b,t]) is the off-diagonal matrix of G([b,t,s])

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The sign problem remains unsolved for V < 0 (attractive interations)!

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