Solution to new sign problems with Hamiltonian Lattice Fermions

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

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- The solution? Fermion bag approach.

The Naive Method

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

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

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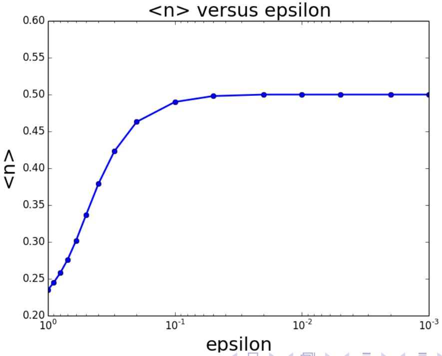
$$\langle n_x \rangle = \frac{\int [d\bar{\psi} d\psi]\, e^{-S} \psi_x \bar{\psi}_x}{\int [d\bar{\psi} d\psi]\, e^{-S}}$$



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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:

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

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

The Partition Function

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

$$\left. e^{-(t_1 - t_2)H_0} \left(s_{x''} n_{x''}^{s_{x''}}\right) \left(s_{y''} n_{y''}^{s_{y''}}\right) \ldots e^{-(t_{k-1} - t_k)H_0} \left(s_{x^{(k)}} n_{x^{(k)}}^{s_{x^{(k)}}}\right) \left(s_{y^{(k)}} n_{y^{(k)}}^{s_{y^{(k)}}}\right) e^{-t_k H_0} \right) \tag{13}$$

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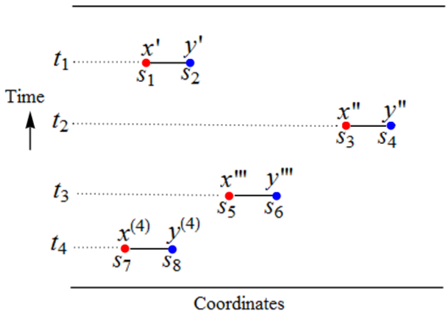

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- The following identities hold: $a_{yx} = -\sigma_x a_{xy} \sigma_y$ and $d_{xx}[s] = -\frac{s_x}{2}$.

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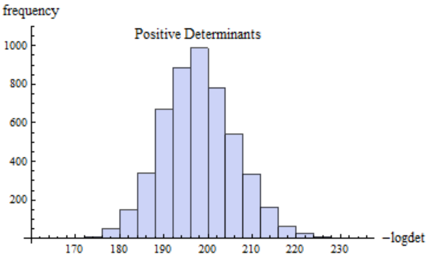

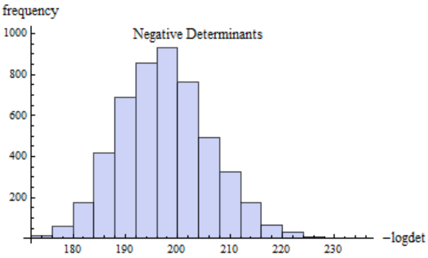

Figure: 10,000 determinants: 5004 were positive and 4996 were negative.

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- We first sum up the diagonal portion.

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- We note that for the diagonal part:

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- Thus our partition function is now given by:

$$Z = \sum_{[b]} \int [dt]\,(-V)^k\, Det\,(A\,([b,t])) \tag{20}$$

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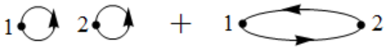

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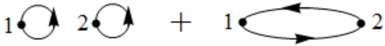
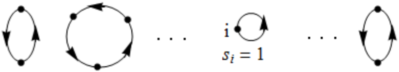


- In our sum of the $D_0 + A$ determinants, for every term of the form



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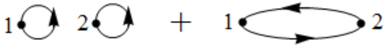
- Alternatively, we can see how this works using the pictorial representation of determinants. For example, a 2×2 determinant can be represented as:



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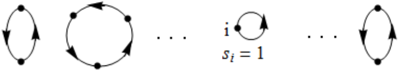

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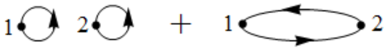

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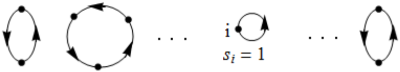

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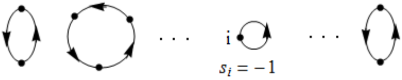

But are the determinants positive?

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

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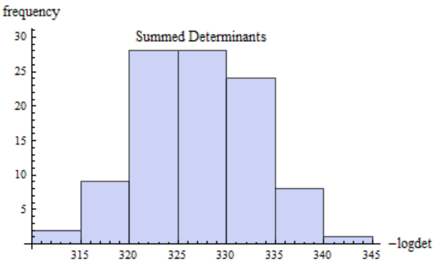
- **We have solved the sign problem. (For repulsive model!)**

Some Example Determinants

- 100 such determinants, randomly selected. All were confirmed to be positive.



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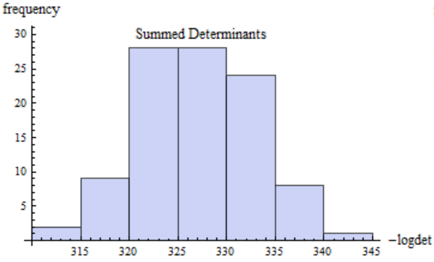
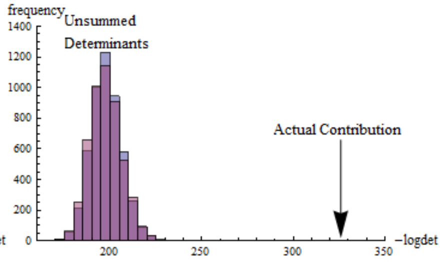
- Note that the probability of positive weight configurations is exponentially smaller, because the -logdet value is larger.





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- Possible to study new quantum critical behavior.