Title: The Fermion Bag Approach in the Hamiltonian Picture

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Abstract: Quantum Monte Carlo methods, when applicable, offer reliable ways to extract the nonperturbative physics of strongly-correlated many-body systems. However, there are some bottlenecks to the applicability of these methods including the sign problem and algorithmic update inefficiencies. Using the t-V model Hamiltonian as the example, I demonstrate how the Fermion Bag Approach--originally developed in the context of lattice field theories--has aided in solving the sign problem for this model as well as aided in developing a more efficient algorithm to study the model. Finally, I discuss some other potential uses for the new algorithm, including for a broader class of models known to be sign-problem-free due to fermion bag ideas.

Fermion Bag Approach in the Hamiltonian Picture

Emilie Huffman
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December 12, 2017

Outline

Motivation

Solving the Sign Problem for the t-V Model

The Fermion Bag Algorithm

Future Outlook

Conclusions

Goals

- Study critical behavior for strongly correlated many-body systems.

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- Study critical behavior for strongly correlated many-body systems.
  1. Expand the family of models where calculations that scale in polynomial time are possible.
  2. Develop more efficient polynomial-time algorithms.

Intro: Quantum Monte Carlo and the Sign Problem

- QMC methods are reliable ways to measure observables.
- Calculation:

$$\langle O \rangle = \frac{\sum_C O(C)\Omega(C)}{\sum_C \Omega(C)}.$$

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- For $\Omega(C) < 0$, often results in a calculation that scales **exponentially** with the system volume.

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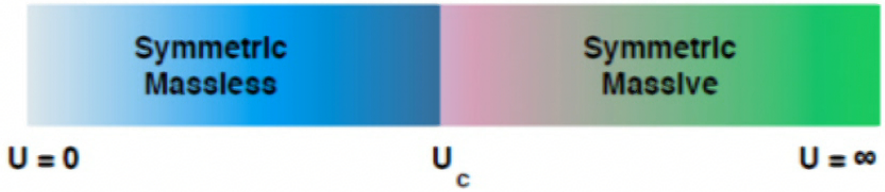
$$S = \frac{1}{2} \sum_{x,\alpha,i=1,2,3,4} \eta_{x,\alpha} \psi_{x,i} \psi_{x+\alpha,i} - U \sum_{x} \psi_{x,1} \psi_{x,2} \psi_{x,3} \psi_{x,4} \qquad (1)$$



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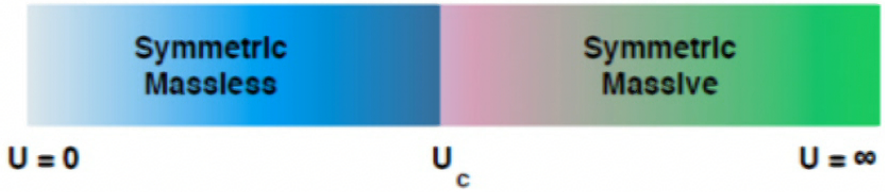

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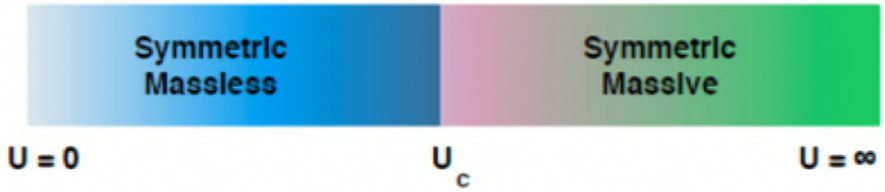

Interesting physics uncovered thanks to large lattice size calculation.

- Wanted to explore models in the Hamiltonian picture.
  Continuous time calculations possible (less fermion doubling).
  Understanding the physics of $N_f = 1$ Dirac fermions.

Auxiliary Field Approach in the Lagrangian Picture

- Auxiliary Field:

$$e^{-U\bar{\psi}_x\psi_y\bar{\psi}_y\psi_x} = \frac{1}{2}\sum_{\sigma_{xy}=\pm 1} e^{\sqrt{U/2}\left(\sigma_{xy}\bar{\psi}_x\psi_y - \sigma_{xy}\bar{\psi}_y\psi_x\right)}$$

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- Partition Function:

$$\begin{aligned} Z &= \int \left[d\bar{\psi}d\psi\right] e^{-S_0\left(\bar{\psi},\psi\right) - U\sum_{xy}\bar{\psi}_x\psi_y\bar{\psi}_y\psi_x} \\ &= \sum_{[\sigma]}\int \left[d\bar{\psi}d\psi\right] e^{-S_0\left(\bar{\psi},\psi\right) - \sqrt{U/2}\left(\sigma_{xy}\bar{\psi}_x\psi_y - \sigma_{xy}\bar{\psi}_y\psi_x\right)} \end{aligned}$$

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- If negative, there is a sign problem.
- Even if positive, $M\left(\sigma\right)$ is nonlocal and may cause inefficiencies.

A Different Approach

- Example: Lattice Thirring model. More efficient calculations (40^3 lattices). (Chandrasekharan, 2010)

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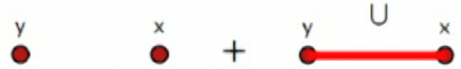
- The expansion terms $1 - U\bar{\psi}_x\psi_y\bar{\psi}_y\psi_x$ pictorially:



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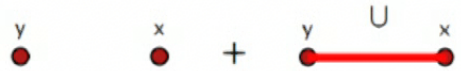
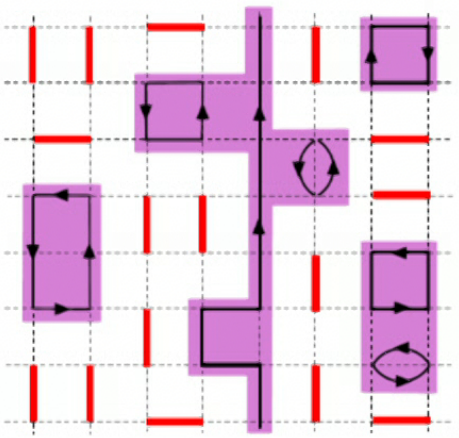


- Re-express the integral, summing over groups of Grassman variables.



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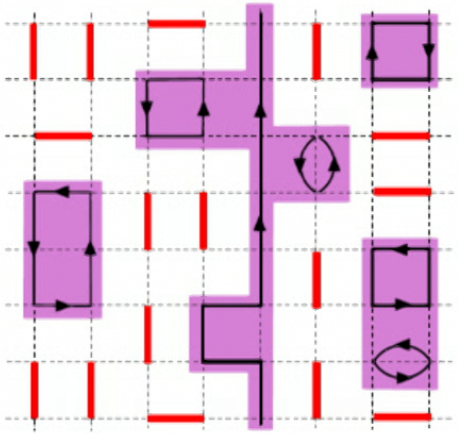
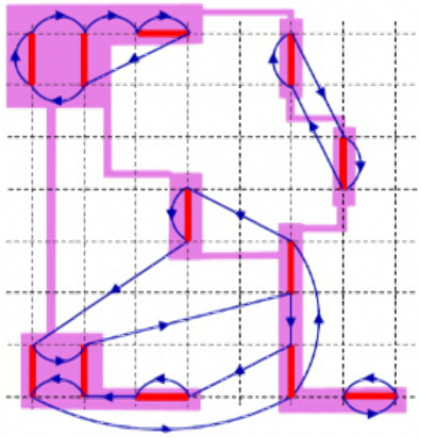
$$Z = \sum_d U^{N_d} \int [d\bar{\psi} d\psi]\, e^{-S_0(\bar{\psi},\psi)} \left(\bar{\psi}_{x_1} \psi_{y_1} \bar{\psi}_{y_1} \psi_{x_1}\right) \ldots \left(\bar{\psi}_{x_k} \psi_{y_k} \bar{\psi}_{y_k} \psi_{x_k}\right)$$

- Strong coupling:



$$Z = \sum_{[s]} U^{N_d} \prod_{\text{Bags}} Det\left(W_{\text{Bag}}\right)$$

- Weak coupling:



$$Z = \sum_{[s]} U^{N_d} \det\left(M\right) \det\left(G_{\text{prop}}\right)$$

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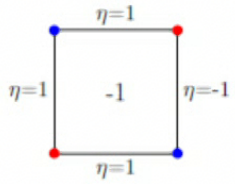

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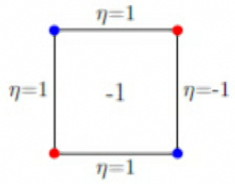

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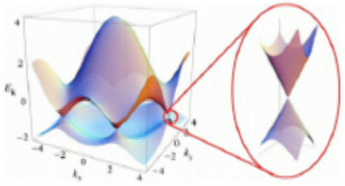

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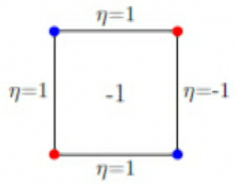

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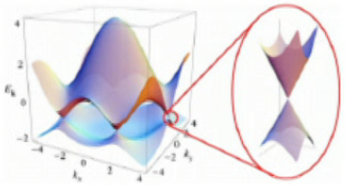

massless fermions — massive fermions

V_c

Exploring the t-V Model

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- What follows is our original solution to the t-V model sign problem.

Solution to the Sign Problem in the t-V Model

- Disclaimer: there is a simpler way to see the solution now, but the following explains how we found it!

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- Inspired by the Lagrangian Fermion Bag approach, take $H_0 = \sum_{\langle xy \rangle} \left(c_x^\dagger c_y + c_y^\dagger c_x \right) = \sum_{\langle x,y \rangle} c_x^\dagger M_{xy} c_y$ and $H_{\text{int}} = \sum_{\langle xy \rangle} (n_x - 1/2)(n_y - 1/2)$,

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$$Z = \sum_k \int_0^\beta dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{k-1}} dt_k (-1)^k \text{Tr} \left(e^{-(\beta - t_k) H_0} H_{\text{int}} \ldots H_{\text{int}} e^{-t_1 H_0} \right)$$

This is known as the CT-INT expansion.

(Beard, Wiese(1996), Sandvik (1998), Prokof'ev, Svistunov (1998), Rubtsov, Savkin, Lichtenstein (2005))

Exploring Hamiltonian Models

- Further expanding H_{int}, we get

$$H_{\text{int}} = \frac{V}{4} \sum_{\langle x,y \rangle} \sum_{s_x, s_y \in \{+,-\}} \left(s_x n_x^{s_x}\right) \left(s_y n_y^{s_y}\right),$$

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- The partition function is then:

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$$\times (-1)^{\sum s} \operatorname{Tr}\left(e^{-(\beta - t_1)H_0} n_{x_1}^{s_{x_1}} n_{y_1}^{s_{y_1}}\right.$$
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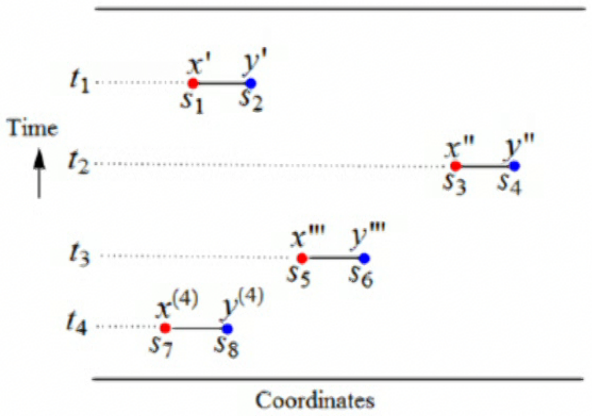

Partition Function Terms

- The usual free particle propagator:

$$\mathrm{Tr}\left(e^{-(\beta-t)H_0}c_x e^{-tH_0}c_y^\dagger\right)/\mathrm{Tr}\left(e^{-\beta H_0}\right)=\left(\frac{e^{-tM}}{\mathbb{1}+e^{-\beta M}}\right)_{xy}$$

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- The formula I derived:

$$(-1)^{\sum s}\,\mathrm{Tr}\left(\ldots\ldots c_x^\dagger c_x e^{-\Delta t H_0} c_y c_y^\dagger \ldots\ldots\right)/\mathrm{Tr}\left(e^{-\beta H_0}\right)$$

$$=\det\begin{pmatrix} \ddots & \vdots & \vdots & \ddots \\ \ddots & -\frac{1}{2} & \left(\frac{e^{-\Delta tM}}{\mathbb{1}+e^{-\beta M}}\right)_{xy} & \ddots \\ \ddots & -\sigma_x\sigma_y\left(\frac{e^{-\Delta tM}}{\mathbb{1}+e^{-\beta M}}\right)_{xy} & \frac{1}{2} & \ddots \\ \ddots & \vdots & \vdots & \ddots \end{pmatrix}$$

The Partition Function

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A\left[b, t\right] &= -DA\left[b, t\right]^T D, \qquad D_{xy} = \sigma_x \delta_{xy}
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$$= \int [dt]\left[d\bar{\psi}d\psi\right] e^{-\bar{\psi}A[b,t]\psi} 4^k$$

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But there are always k odd sites, so $(-1)^k = \prod_q^{2k} \sigma_q = \det D$.

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$$\det \left(A \, [b, t] \, D \right) \geq 0. \tag{5}$$

- No sign problem!

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- A simpler way to see our result (Li, Jiang and Yao (2014), Wei, Wu, Li, Zhang and Xiang (2016)).

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- We get two commuting Hilbert spaces and can express Z as

$$Z = \sum_{\{C\}} \mathrm{Pf}\left(\mathrm{A}\left(\mathrm{C}\right)\right)^2 = \sum_{\{C\}} \det\left(\mathrm{A}\left(\mathrm{C}\right)\right). \tag{8}$$

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FRG (linear cutoff) [10,11]	0.927	0.525
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[18] L. Wang, P. Corboz, and M. Troyer, New J. Phys. **16**, 103008 (2014).

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- Lattice sizes ranged from 484 sites to 576 sites on the π-flux lattice. Could we do bigger lattices?

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- Write:

$$H = -\sum_{\langle xy \rangle} \delta e^{2\alpha \left(c_x^\dagger c_y + c_y^\dagger c_x \right)} = -\sum_{\langle xy \rangle} H_{xy} \qquad (9)$$

where

$$\delta = \frac{V^2}{t} \left(1 - (V/2t)^2 \right),$$

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- Related to SSE expansion. (Wang, Liu, Troyer (2016))

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$$Z = \sum_{k,\{\langle x,y\rangle\}} \int_0^\beta dt_1 \int_0^{t_1} dt_2 ... \int_0^{t_{k-1}} dt_k \, \mathrm{Tr}\left(H_{x_k y_k} ... H_{x_2 y_2} H_{x_1 y_1}\right).$$

- Our formula shows these terms are positive, and also the Majorana fermion transformation:

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and a $2k \times 2k$ Pfaffian squared:

$$\mathrm{Tr}\left(H_{x_k y_k} ... H_{x_2 y_2} H_{x_1 y_1}\right) = \mathrm{Pf}\left(a\left[x, y, k\right]\right)^2.$$

Calculating the terms

- So, we know there is a way to calculate the traces using $2k \times 2k$ matrices.

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- Instead, we use the BSS formula, a key to Hamiltonian auxiliary field methods.

Hamiltonian Auxiliary Field Approach

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Blancenbecler, Scalapino, Sugar, 1981

Nonlocal and Local

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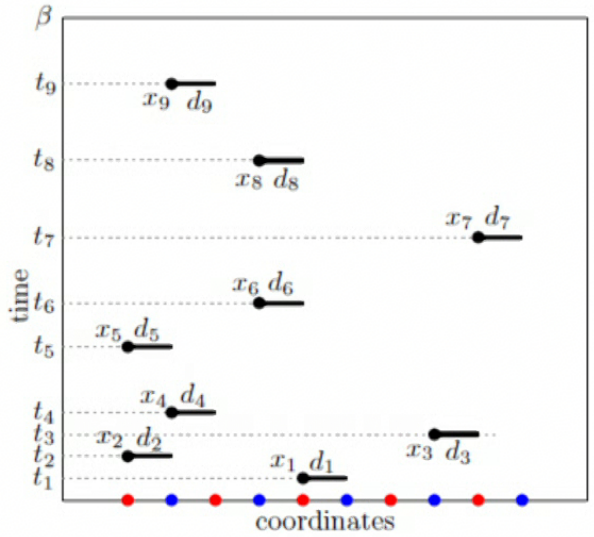

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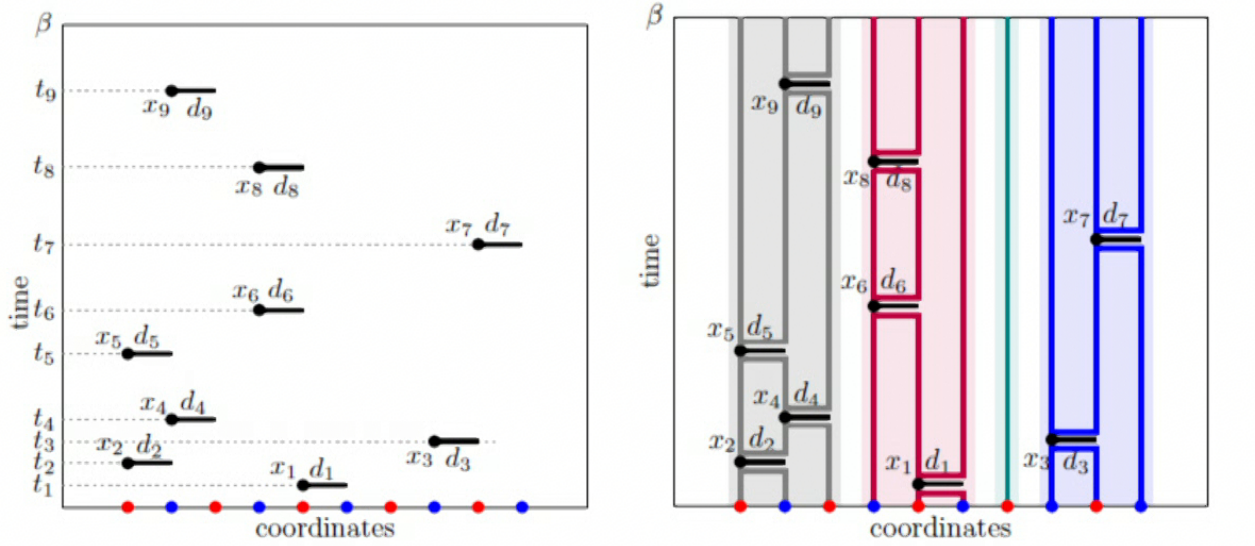
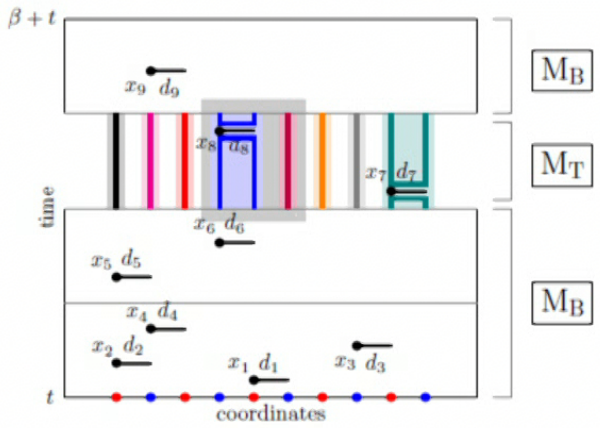


Fermion Bags



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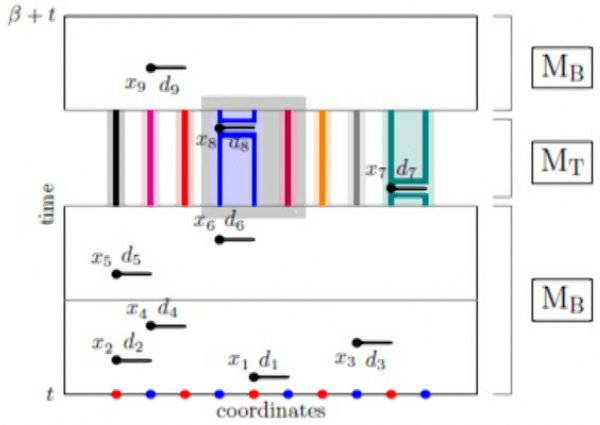

- Sweep: Every timeslice updated, linearly in time. (βL^6)

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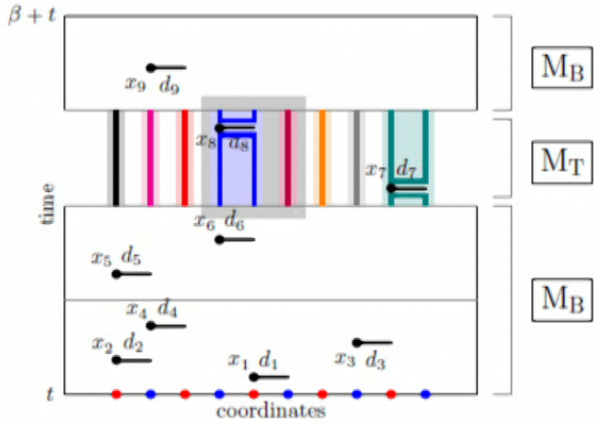

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$$= \det\left(\mathbb{1} + B_{x_k y_k} \ldots B_{x_2 y_2} B_{x_1 y_1}\right)$$

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M_T matrices are products of B_{xy} matrices.

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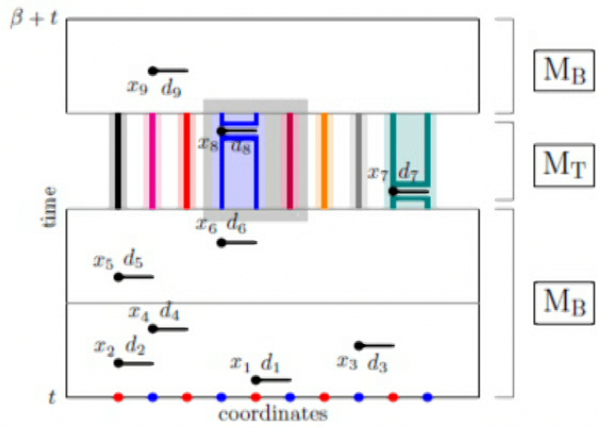

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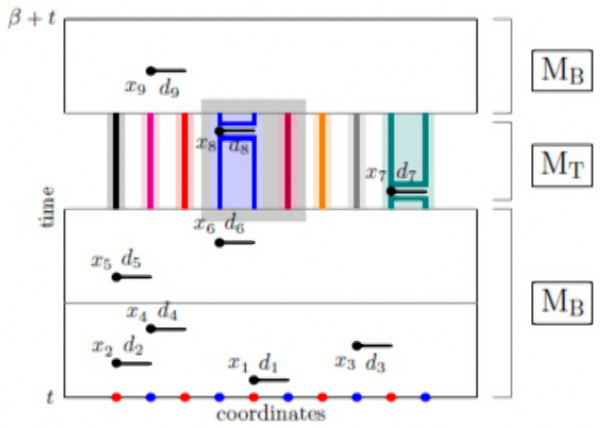
- Sweep: Every timeslice updated, linearly in time. (βL^6)
- Updates:

$$R = \det\left(\mathbb{1} + G_B \Delta\right),$$

$$G_B = \left(\mathbb{1} + M_B M_T\right)^{-1} M_B M_T.$$

Determinants of matrices with dimensions on the order of fermion bag size.

Fermion Bags



$$\mathrm{Tr}\left(H_{x_k y_k} \ldots H_{x_2 y_2} H_{x_1 y_1}\right)$$

$$= \det\left(\mathbb{1} + B_{x_k y_k} \ldots B_{x_2 y_2} B_{x_1 y_1}\right)$$

$$= \det\left(\mathbb{1} + M_B M_T\right)$$

M_T matrices are products of B_{xy} matrices.

- Sweep: Every timeslice updated, linearly in time. (βL^6)
- Updates:

$$R = \det\left(\mathbb{1} + G_B \Delta\right),$$

$$G_B = \left(\mathbb{1} + M_B M_T\right)^{-1} M_B M_T.$$

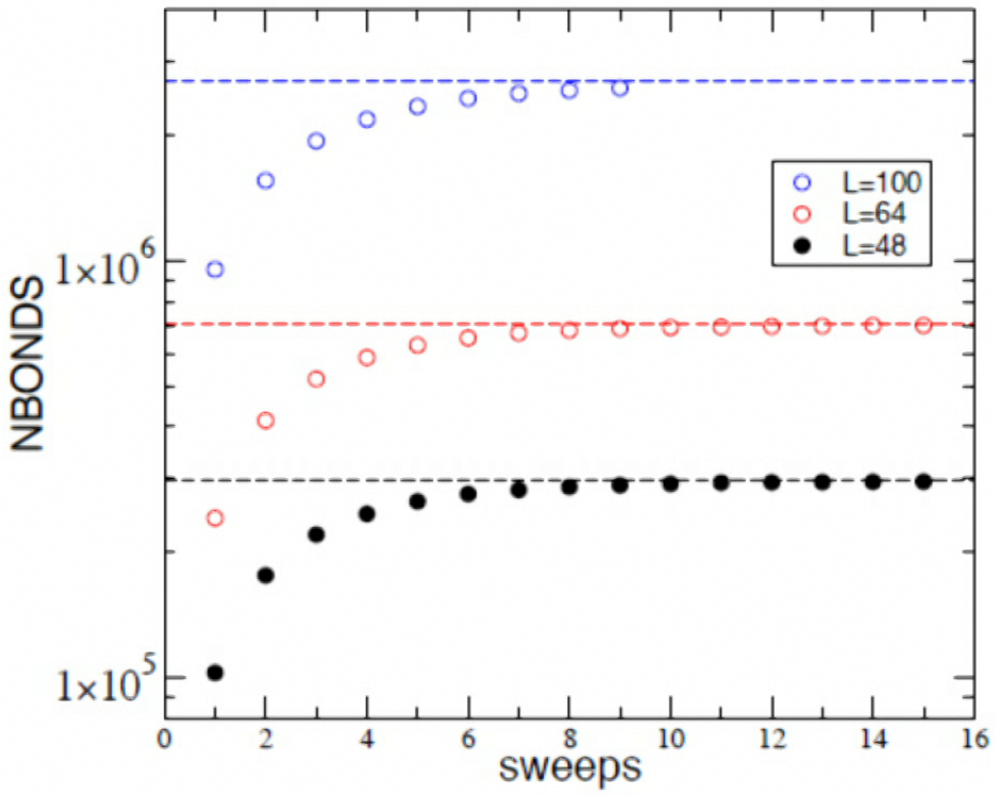
Determinants of matrices with dimensions on the order of fermion bag size.

- Stabilization:

$$\left(\mathbb{1} + M_1 M_2\right)^{-1} =$$
$$G_1 \left(G_1 G_2 + \left(\mathbb{1} - G_1\right)\left(\mathbb{1} - G_2\right)\right)^{-1} G_2,$$

$$G_i = \left(\mathbb{1} + M_i\right)^{-1}.$$

Equilibration $\beta = L$



Results

- Choosing $\beta = L$ we use the equal time density-density correlation function as an order parameter:

$$\langle C \rangle = \sigma_0 \sigma_{L/2} \left\langle (n_0 - 1/2) \left(n_{L/2} - 1/2 \right) \right\rangle \qquad (12)$$

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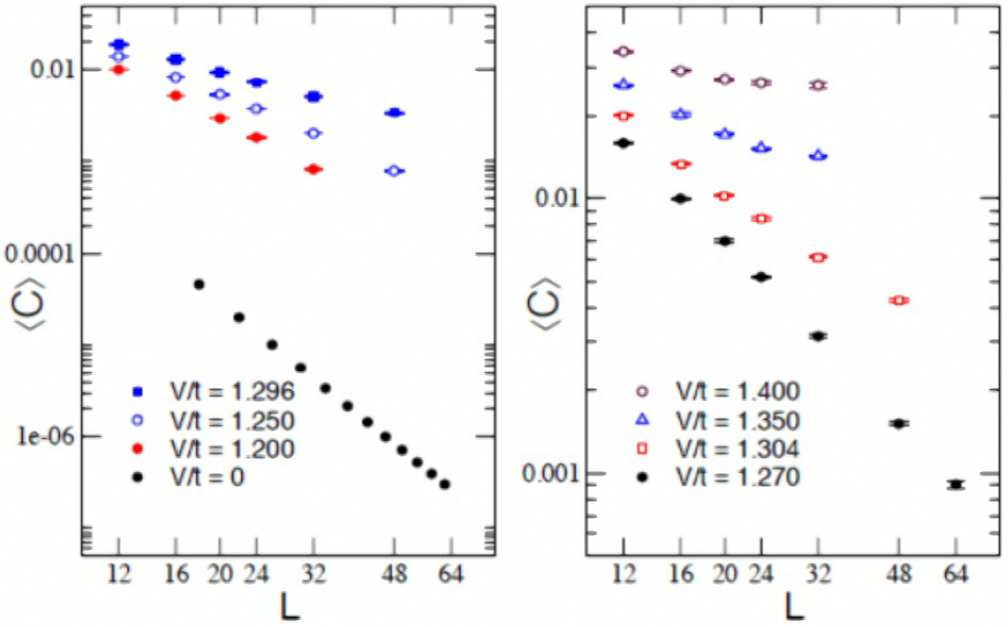
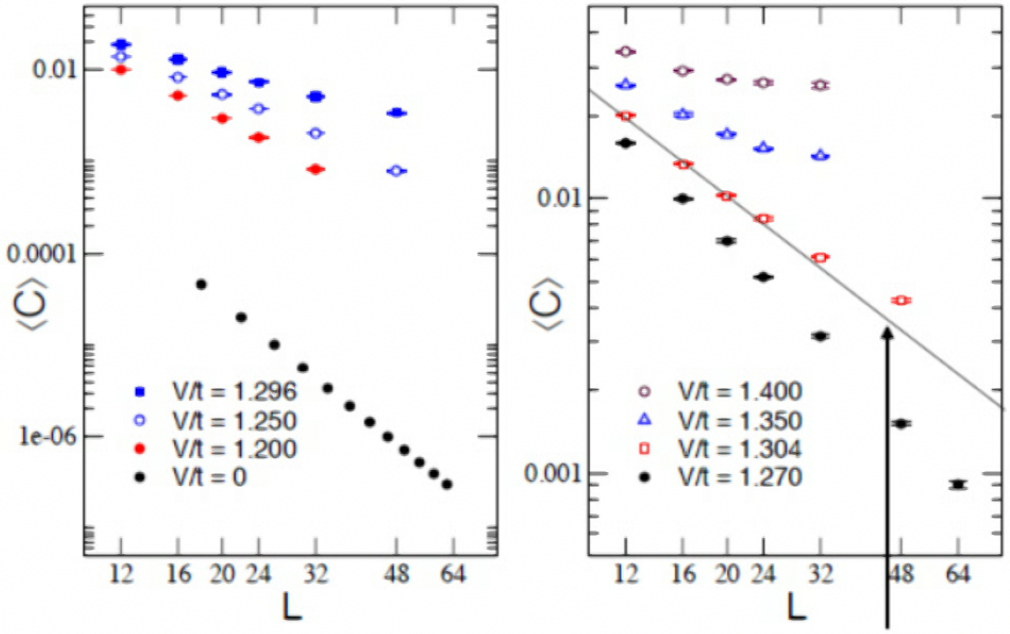
- massless (semimetal) fermion phase: $\langle C \rangle \sim \frac{1}{L^4}$
- massive (insulator) fermion phase: $\langle C \rangle \sim \text{const.}$

Our Results


0.01
0.0001
1e-06
⟨C⟩
V/t = 1.296
V/t = 1.250
V/t = 1.200
V/t = 0
12 16 20 24 32 48 64
L
0.01
0.001
⟨C⟩
V/t = 1.400
V/t = 1.350
V/t = 1.304
V/t = 1.270
12 16 20 24 32 48 64
L

Our Results



- Wang, Carboz and Troyer, 2014
  (484 sites)
  $\nu = 0.80(2), \eta = .30(1).$

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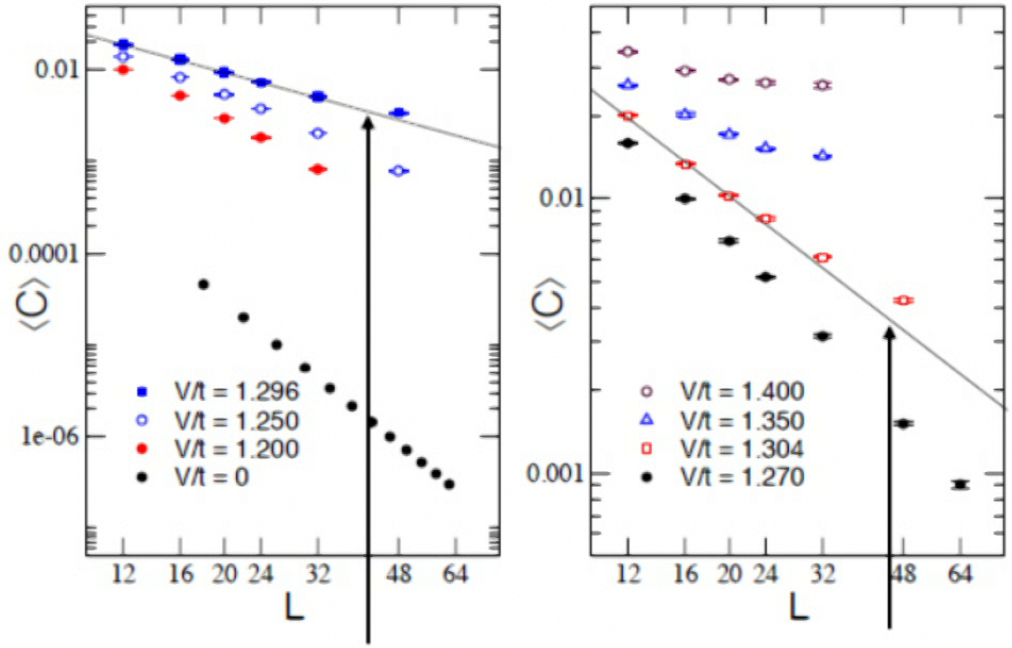
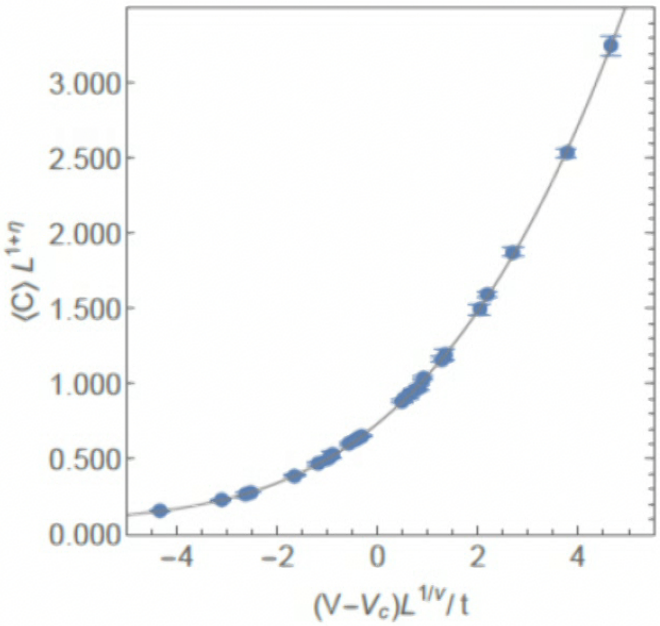


- Li, Jiang and Yao, 2014 (576 sites)
  $\nu = 0.77(3), \eta = 0.45(2).$
- Wang, Carboz and Troyer, 2014
  (484 sites)
  $\nu = 0.80(2), \eta = .30(1).$

Critical Scaling

$$\langle C \rangle = \frac{1}{L^{1+\eta}} f\left((V - V_c)\, L^{1/\nu} / t \right)$$



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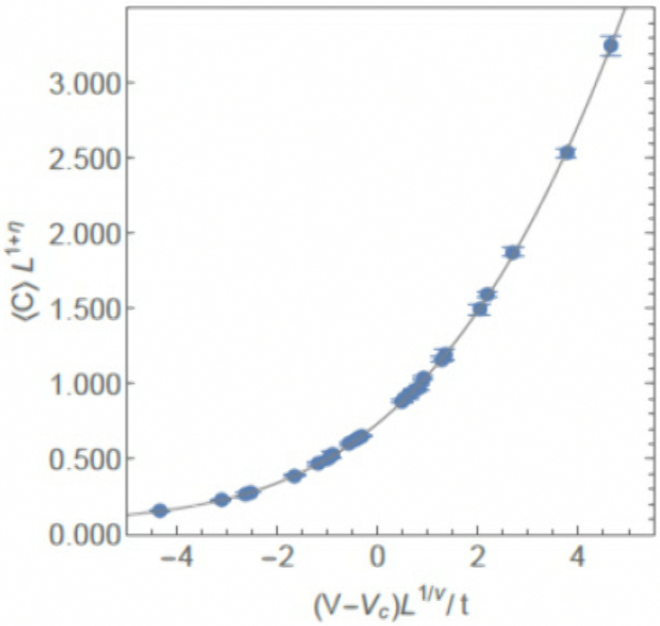

$$f(x) = f_0 + f_1 x + f_2 x^2 + f_3 x^3$$

- $V_c/t = 1.279(3), \qquad \eta = 0.54(6), \qquad \nu = 0.88(2), \qquad \chi^2/DOF \sim 0.8$

Future Outlook

- Fermion bags methods helpful for solving sign problems in these fermion-boson interacting models. Not obvious if auxiliary fields work. (EH and Chandrasekharan (2016))

$$H = -t \sum_{\langle ij \rangle} \left(c_i^\dagger c_j + c_j^\dagger c_i \right) + V \sum_{\langle ij \rangle} \left(n_i - \frac{1}{2} \right) \left(n_j - \frac{1}{2} \right) + J \sum_{ij} S_i \cdot S_j - \sum_i h_i \left(n_i - \frac{1}{2} \right) S_i^x \tag{13}$$

Future Outlook

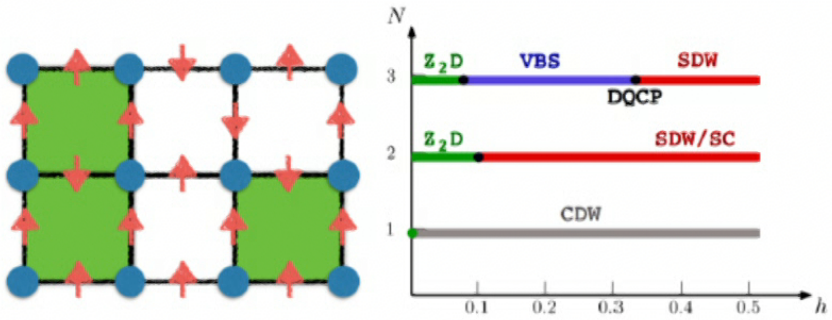

Figure: Gazit, Randeria, Vishwanath (2017), Assaad and Grover (2016)

- Family of Hamiltonians with $\mathbb{Z}_2$ gauge symmetries:

$$H = -t \sum_{\langle x,y\rangle,\sigma} \left(\sigma^3_{x,y} c^\dagger_{x,\sigma} c_{y,\sigma} \right) \pm h \sum_{\langle x,y\rangle} \sigma^1_{x,y} \qquad (14)$$

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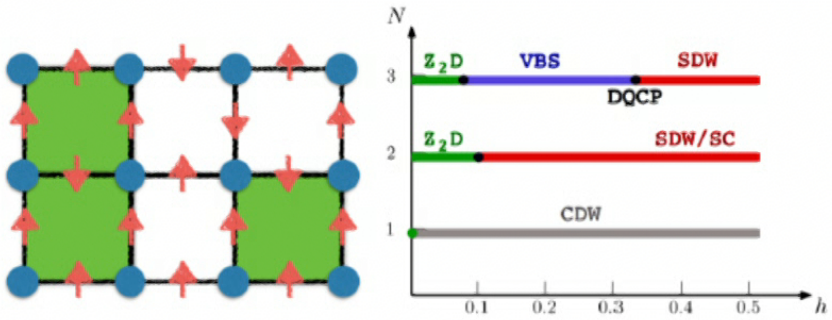

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- Continuous transitions offer both symmetry breaking and a confinement of the gauge field.
- Largest lattices simulated so far: L=16 (256 sites).
- Auxiliary fields limited in efficiency for these models.

Conclusions

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- The Fermion Bag algorithm has been demonstrated to be effective in Hamiltonian models, with stable calculations at large lattices a possibility.
- New opportunities to study quantum critical points.