Fermion Bag Approach to Lattice Hamiltonian Field Theories

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Motivation for Hamiltonian Approach

- Lattice Hamiltonian approach often especially useful for studying strongly correlated 2D materials with massless Dirac fermions at low energies.

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- Example: Repulsive Hubbard model on honeycomb lattice

$$H = \sum_{\langle xy \rangle, \sigma} -t \left(c^\dagger_{x,\sigma} c_{y,\sigma} + c^\dagger_{y,\sigma} c_{x,\sigma} \right) + U \sum_i \left(n_{i,\uparrow} - 1/2 \right) \left(n_{i,\downarrow} - 1/2 \right),$$

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- This model has an additional SU(2) symmetry that is broken at the critical point, but the Lagrangian $N_f = 2$ staggered fermions with a four-fermi term do not.

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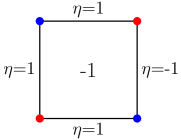
describes $N_f = 1$, 4-component Dirac fermions.

($\eta_{xy} = \pm 1$ is a bond dependent π-flux term)



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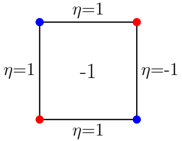

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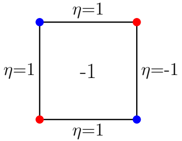

- We also get one flavor of massless Dirac fermions using reduced staggered fermions in the Lagrangian approach.
- But, the interaction term causes a sign problem in the Lagrangian approach that does not exist in the Hamiltonian approach. (E.H. and Chandrasekharan, Phys. Rev. B. (2014)

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Method	ν	η
$4-\epsilon$, first order [9]	0.709	0.577
$4-\epsilon$, second order [9]	0.797	0.531
FRG (linear cutoff) [10,11]	0.927	0.525
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FRG [13]	0.929	0.602
$1/N$ expansion [11]	0.738	0.635
CT-INT (GS) [18]	0.80(3)	0.302(7)
MQMC (GS) [19]	0.77(3)	0.45(2)
LCT-INT (GS) [20]	0.80(3)	0.302(7)
CT-INT (finite T), here	0.74(4)	0.275(25)

[18] L. Wang, P. Corboz, and M. Troyer, New J. Phys. 16, 103008 (2014).

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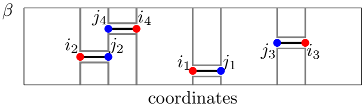
- CT methods say $\eta = .3$, but discrete method uses slightly larger lattices and says $\eta = .45$. Can we go to even larger lattices?

Fermion Bag Method

- We expand out (at least the higher order) exponentials of the fermions in our sum, and for each configuration we divide the lattice space into smaller, factorizable regions, dependent on the configuration.

$$e^{U\prod_{x,y}\bar{\psi}_x\psi_x\bar{\psi}_y\psi_y} = \sum_{n_p=0,1}\left(U\prod_{x,y}\bar{\psi}_x\psi_x\bar{\psi}_y\psi_y\right)^{n_p} \quad (1)$$

Chandrasekharan Eur. Phys. J. A (2013)



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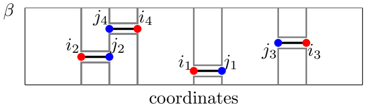

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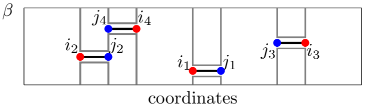

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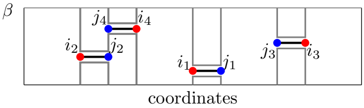

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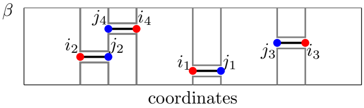

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  - Local Factorization, Ce, Giusti, Schaefer (2016). (plenary on Monday)

Fermion Bag method and Stochastic Series Expansion

- To apply the Fermion Bag idea to $N_f = 1$, we use the Stochastic Series expansion, where the partition function can be expanded in terms of *local* insertions:

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right) = \sum_{k,\{\langle xy\rangle\}} \int [dt]\,(-1)^k\,\mathrm{Tr}\left(H_{x_1 y_1} H_{x_2 y_2} \ldots H_{x_k y_k}\right).$$

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- This model in particular, given by

$$H = \sum_{\langle xy\rangle} \left[-t\eta_{xy}\left(c_x^\dagger c_y + c_y^\dagger c_x\right) + V\left(n_x - 1/2\right)\left(n_y - 1/2\right)\right]$$
$$= \sum_{\langle xy\rangle} H_{xy},$$

has the nice property that up to a constant, we can write

$$H_{xy} = -\delta e^{2\alpha\left(c_x^\dagger c_y + c_y^\dagger c_x\right)},$$

where α and δ can be found in terms of t and V. Because we have exponential pieces, we can use the BSS formula.

Blankenbecler, Scalapino, Sugar (1981)

The BSS Formula

- With the BSS formula, we can write the partition function as

$$Z = \sum_{k,\{\langle xy \rangle\}} \int [dt]\,(-1)^k \delta^k \det\left(\mathbb{1} + B_{x_1 y_1} B_{x_2 y_2} \ldots B_{x_k y_k}\right) \quad (2)$$

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- The B_{xy}-matrices are of the form $P\left(\mathbb{1}_{N-2} \otimes A\right) P$, where N is the number of sites, P are permutation matrices and

$$A = \begin{pmatrix} \cosh 2\alpha & \eta_{xy} \sinh 2\alpha \\ \eta_{xy} \sinh 2\alpha & \cosh 2\alpha \end{pmatrix}. \quad (3)$$

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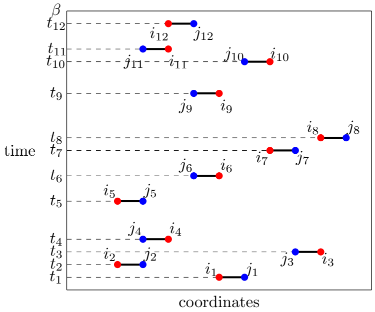
- Importantly

$$\left[B_{xy}, B_{x'y'} \right] = 0, \quad (4)$$

  if $x \neq x'$ and $y \neq y'$.

Visualizing the Fermion Bag Idea

- We can make a diagram to represent the partition function, with nearest neighbor bonds representing H_{xy} inserted within imaginary time.



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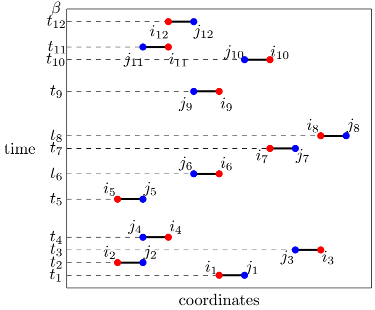
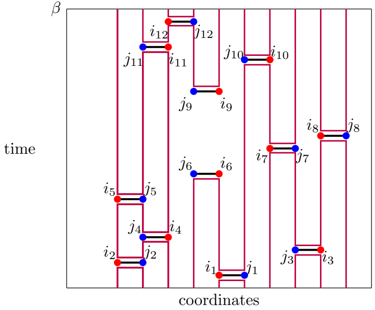
- We can make a diagram to represent the partition function, with nearest neighbor bonds representing H_{xy} inserted within imaginary time.
- For this diagram, all of the bonds can be connected because they share sites in common. They form one fermion bag.





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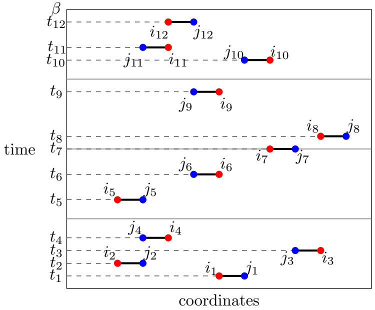

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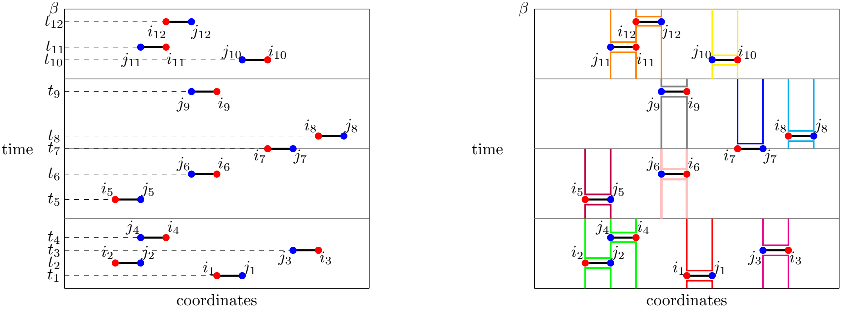

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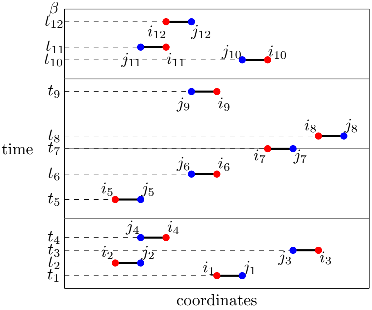

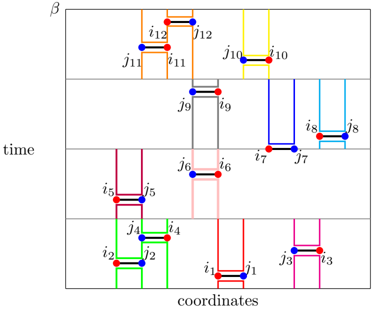

- The *B*-matrices in a cluster will commute with *B*-matrices belonging to any other cluster in a timeslice.

Maximum Fermion Bag Size and Equilibration

- We find that for a timeslice of .25, fermion bags are no bigger than around 30 sites. This holds across lattice sizes.

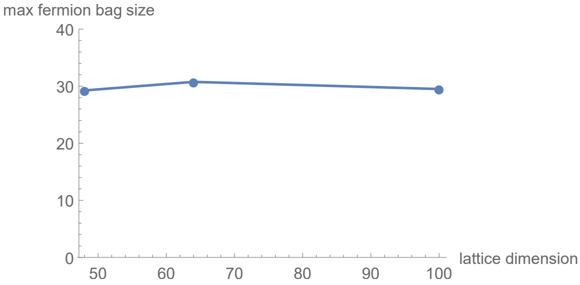

Figure: Average maximum sizes of clusters in each timeslice for equilibrated configurations. Timeslice size is .25.

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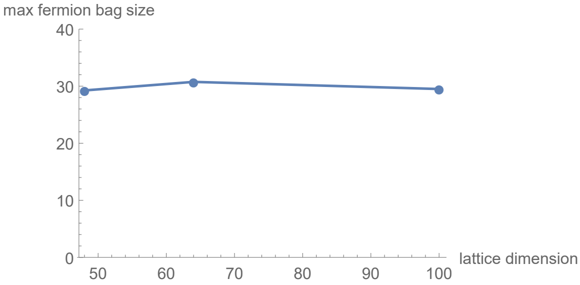
- We can often then calculate weight ratios then as determinants of 30×30 matrices or smaller.



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Stabilization Method

- To get the determinantal weight ratios w_1/w_2, we must calculate:

$$G = \left(\mathbb{1} + B_{x_1 y_1} B_{x_2 y_2} \ldots B_{x_k x_k}\right)^{-1}, \tag{5}$$

because

$$w_1/w_2 = \det\left(\mathbb{1} + (1 - G)\left(M_{\mathrm{FB}}^{-1} M'_{\mathrm{FB}} - \mathbb{1}\right)\right)_{\mathrm{FB}\times\mathrm{FB}}, \tag{6}$$

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$$\times \left((\mathbb{1} + M_1)^{-1} (\mathbb{1} + M_2)^{-1} + (\mathbb{1} + M_1)^{-1} M_1 M_2 (\mathbb{1} + M_2)^{-1}\right)^{-1} (\mathbb{1} + M_1)^{-1}$$

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$$G = \left(\mathbb{1} + B_{x_1y_1} B_{x_2y_2} \ldots B_{x_kx_k}\right)^{-1}, \qquad (5)$$
because
$$w_1/w_2 = \det\left(\mathbb{1} + (1 - G)\left(M_{\mathrm{FB}}^{-1} M'_{\mathrm{FB}} - \mathbb{1}\right)\right)_{\mathrm{FB}\times\mathrm{FB}}, \qquad (6)$$
where the dimension of the determinant is reduced from *Vol*. $\times$ *Vol*. and related to the sizes of the fermion bags (*FB*).
- At equilibration, we can have hundreds of thousands of B_{xy} matrices, leading to stabilization issues.
- Traditionally, SVD factorization has been used for stabilization.
- Instead, we use the formula
$$\left(\mathbb{1} + M_1 M_2\right)^{-1} = \left(\mathbb{1} + M_2\right)^{-1}$$
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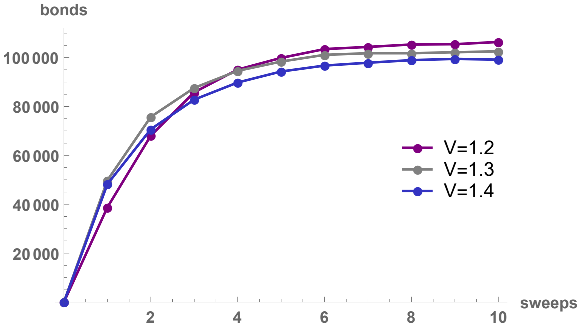

Figure: Equilibration of t-V model on a square 100×100 lattice. ($\beta = 4.0$)

- The observable is the average number of bonds $\langle n \rangle = -\beta \langle H \rangle + \beta N_b t^2 / V$.

Scaling of time: Pi-Fluxes near Critical Point

- This algorithm has scaling βN^3 in accordance with *LCT-INT* algorithms, as opposed to $\beta^3 N^3$ for *CT-INT*-algorithms. (Wang, Iazzi, Corboz, Troyer, PRB 91 (2015))

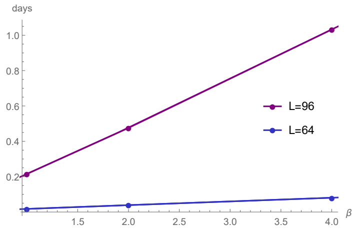

Figure: Time to do one sweep for different β values at $V = 1.304$.

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- We can see the linear scaling in time at small β-values and extrapolate for the time of a full sweep at large β. (times based on a single thread–multithreaded LAPACK libraries speed up by at least a factor of 2)

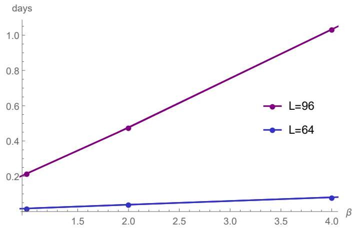

Figure: Time to do one sweep for different β values at $V = 1.304$.

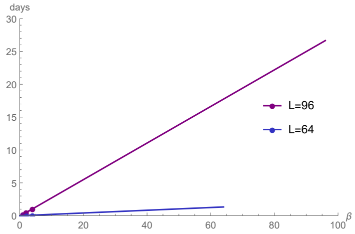

Figure: Extrapolation to low temperatures.

Calculation of η-exponent

- We know that $\langle O \rangle = \frac{1}{L^{1+\eta}} f\left[(V - V_c) L^{1/\nu}\right]$, where V_c is the critical coupling. If we set $V = V_c$, we should get a power law decay. ($O = \langle \sigma_0 \sigma_p (n_0 - 1/2)(n_p - 1/2) \rangle$)

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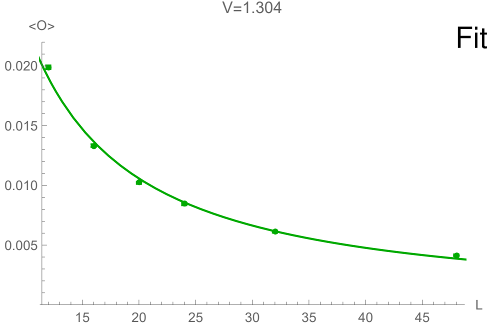
- Assuming that $V_c = 1.304$ as in the CT-INT calculation leads to large χ^2 and discrepancy with calculated value of $\eta = .302(7)$ when larger lattices are included. Results consistent when only up to $L = 20$ included.

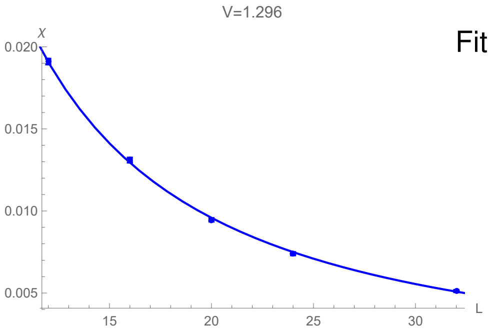


Fit:

$$y\left(x\right) = a_1 x^{a_2}$$
$$a_1 = .330(9)$$
$$a_2 = -1.149(9)$$
$$\chi^2 = 21.47$$
$$\eta = .149(9)$$

Calculation of η-exponent (cont.)

- But assuming, on the other hand, that $V_c = 1.296$ as in the auxiliary field method, leads to a discrepancy with the calculated value of $\eta = .45(2)$.



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$$\chi^2 = 1.114$$
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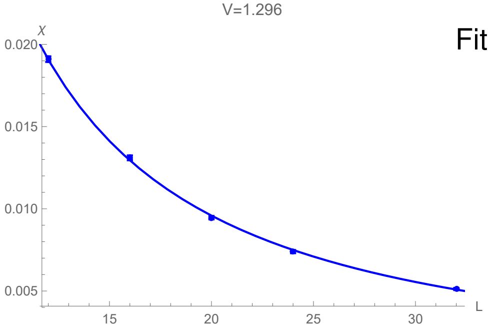

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- Our preliminary results from a combined fit (including seven different couplings and lattice sizes up to 48 for some of them) are $V_c = 1.286(2)$ and $\eta = .45(2)$. Again, our results are consistent with previous results if only lattices up to $L = 20$ are considered.

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- Larger lattices than currently in the literature seem to be important to resolve the η.
- We have also shown the potential of this method for stable calculation at even larger lattices (64×64, 100×100) than we have explored so far.