Fermion Bag Solutions to Sign Problems

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in collaboration with Anyi Li

The QCD Sign Problem

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The QCD partition function

$$Z = \int [dU]\, e^{-S_G(U)} \quad \int d\overline{\psi}\; d\psi e^{-\overline{\psi}_x M_{xy}[U,U^\dagger]\;\psi_y}$$

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solvable form

In the presence of a chemical potential

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Loss of “pairing” is the origin of the sign problem

Sign Problems in Yukawa Models

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Consider the partition function

$$Z = \int [dU]\ e^{-S_G(U)} \int [d\phi]\ e^{-S_b(\phi)} \int d\overline{\psi}\ d\psi e^{-\overline{\psi}_x M_{xy}[U,U^\dagger]\ \psi_y - g\phi_x \overline{\psi}_x \psi_x}$$

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The fermion matrix is now given by

$$(\phi + M[U,U^\dagger]) \;=\; \begin{pmatrix} g\varphi_e & D[U,U^\dagger] \\ -(D[U,U^\dagger])^\dagger & g\varphi_o \end{pmatrix}$$

where $\varphi_e, \;\; \varphi_o$ are diagonal complex matrices.

Again, $Det(\phi + M[U, U^\dagger])$ is not guaranteed to be positive.

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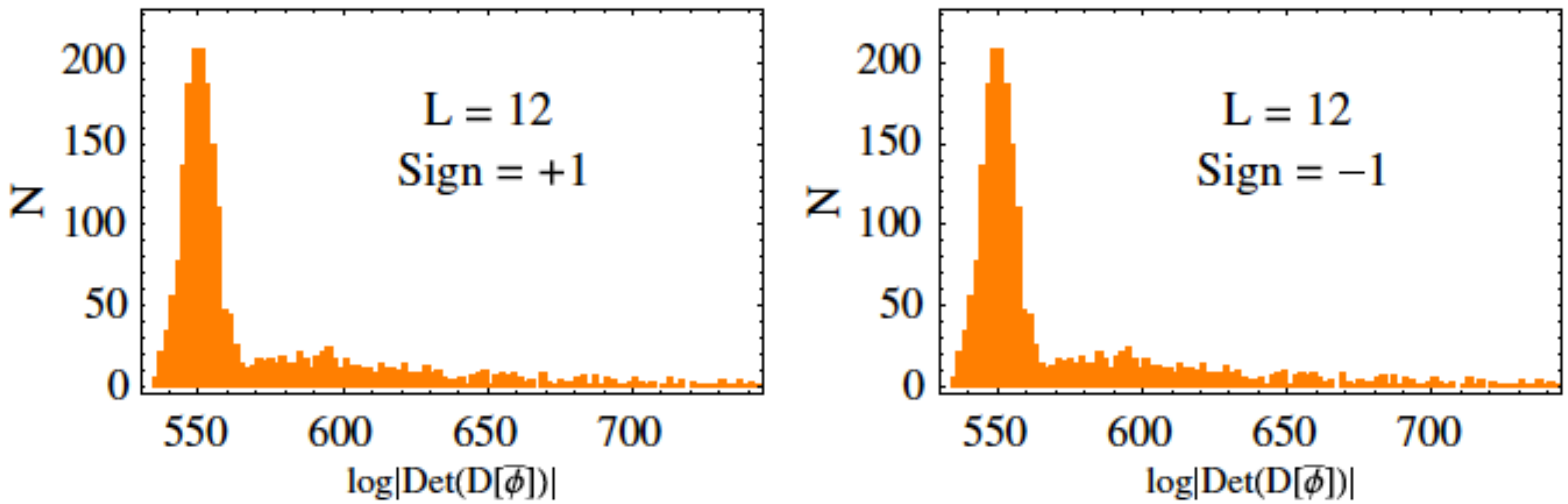

sign problem with fluctuating mass
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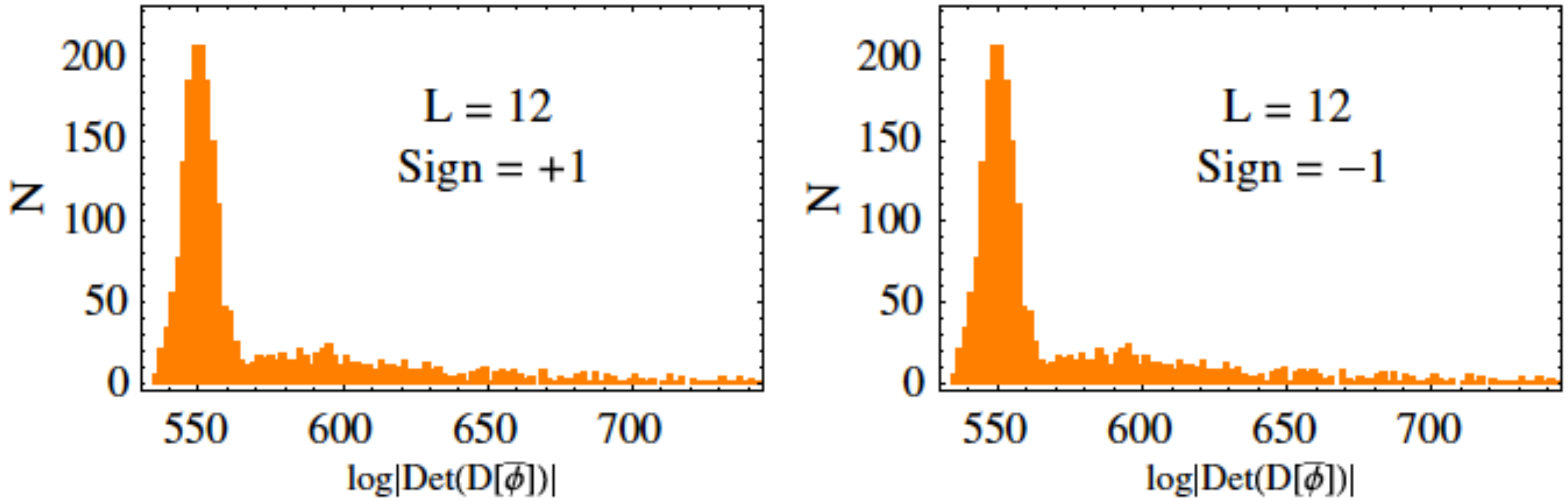

sign problem with fluctuating mass with N=1 staggered fermions

The Yukawa coupling can also destroy the “pairing” mechanism

Take Home Lessons

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A new class of “Yukawa” sign problems are now solvable using the “fermion bag approach”.

The Fermion Bag Idea

SC, 2010

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Group Fermion Worldlines
(fermion bags)
and sum over each group individually.

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Choose fermion bags carefully
that help solve sign problems

Consider

$$\int [d\overline{\psi} d\psi] \; e^{-\overline{\psi}_i M_{ij} \psi_j} \; (-\overline{\psi}_{i_1} \psi_{i_1})(-\overline{\psi}_{i_2} \psi_{i_3} \overline{\psi}_{i_3} \psi_{i_2})$$

$$(-\overline{\psi}_{i_2} \psi_{i_3} \overline{\psi}_{i_3} \psi_{i_2}) \; (-\overline{\psi}_{i_4} \psi_{i_4})(-\overline{\psi}_{i_5} \psi_{i_5})$$

$$(-\overline{\psi}_{i_6} \psi_{i_7} \overline{\psi}_{i_7} \psi_{i_6}) \quad (-\overline{\psi}_{i_8} \psi_{i_9} \overline{\psi}_{i_9} \psi_{i_8})$$

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$$\int [d\overline{\psi} d\psi]\ e^{-\overline{\psi}_i M_{ij} \psi_j}\ (-\overline{\psi}_{i_1}\psi_{i_1})(-\overline{\psi}_{i_2}\psi_{i_3}\overline{\psi}_{i_3}\psi_{i_2})$$

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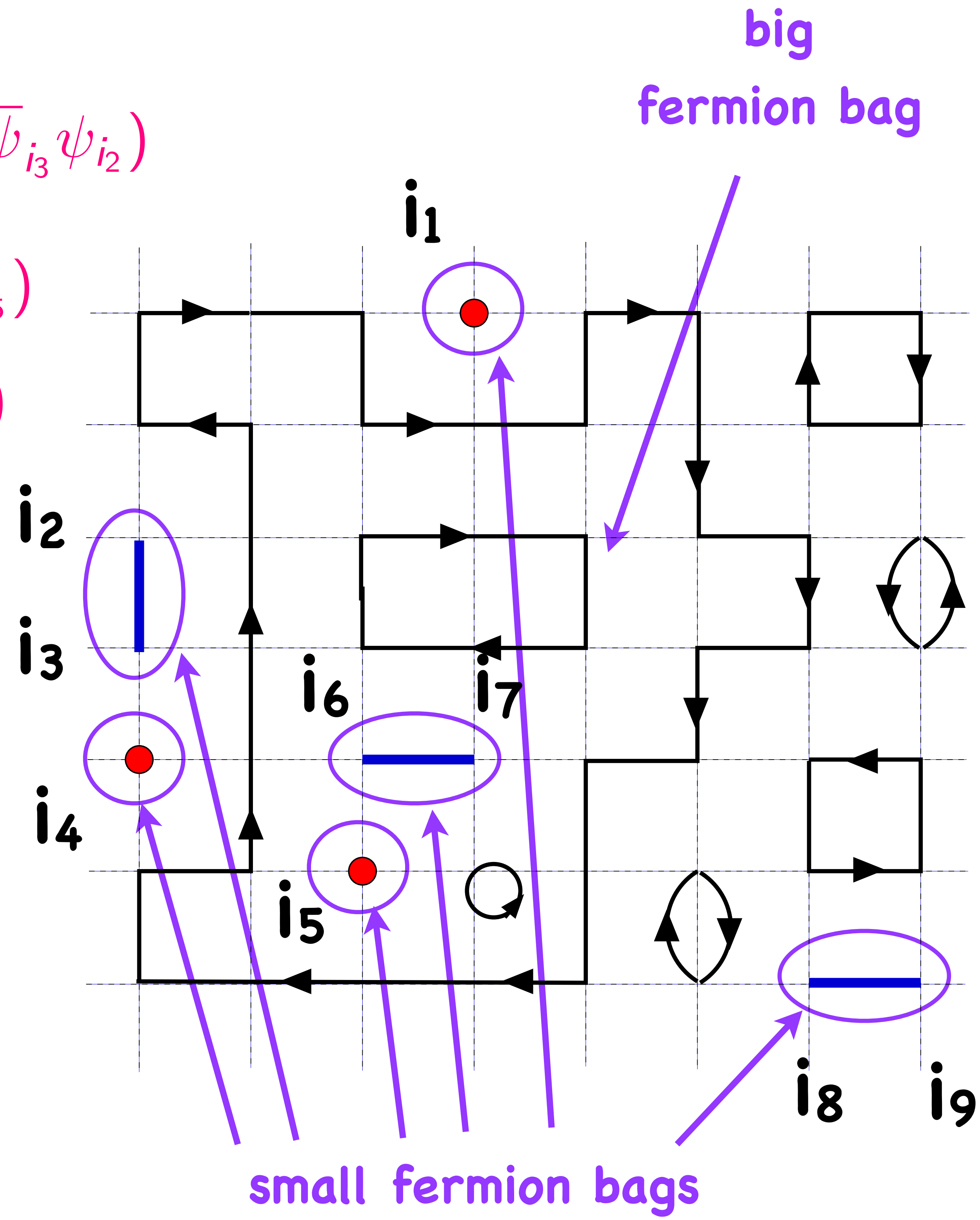

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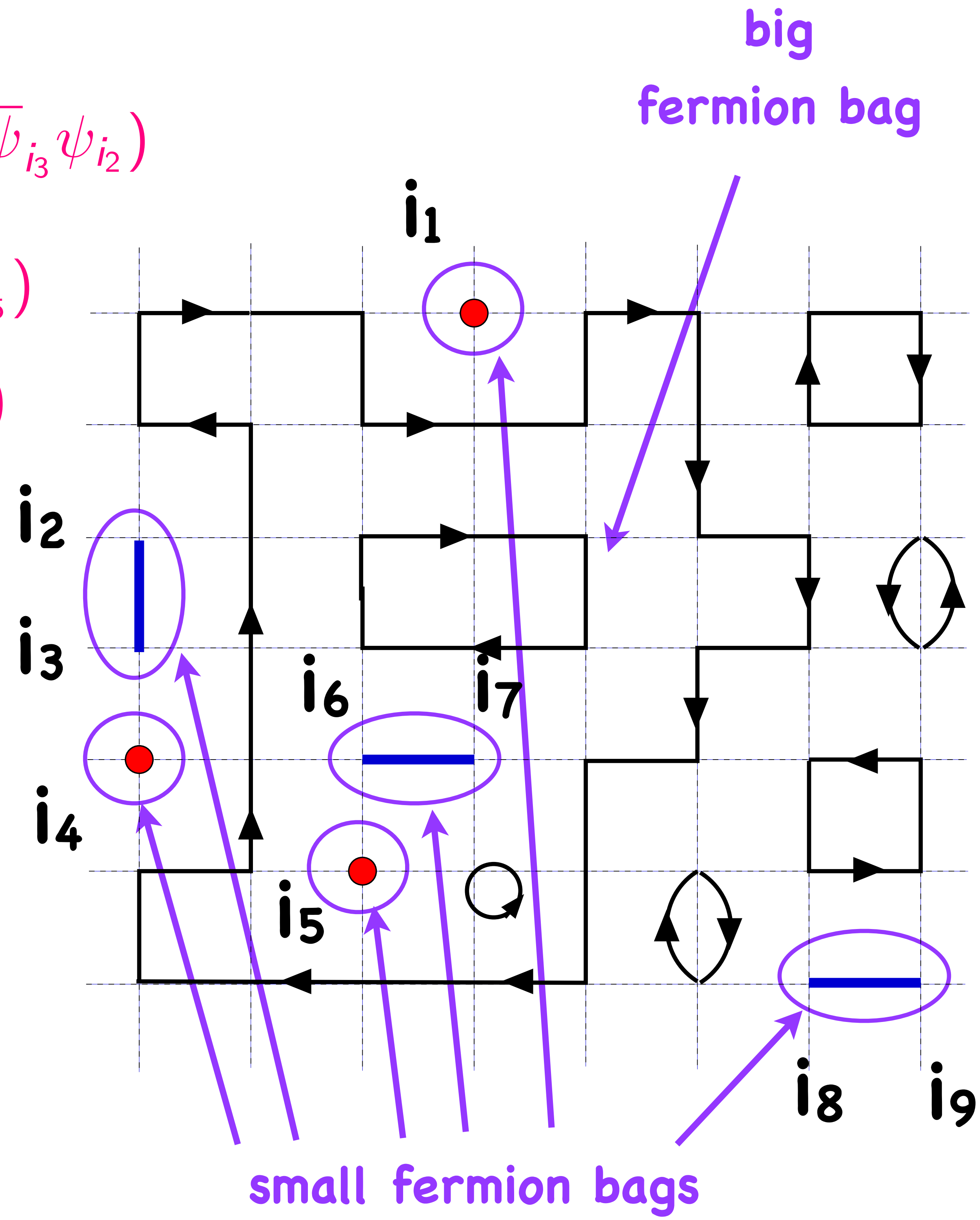
$$=\ \mathrm{Det}(W)$$



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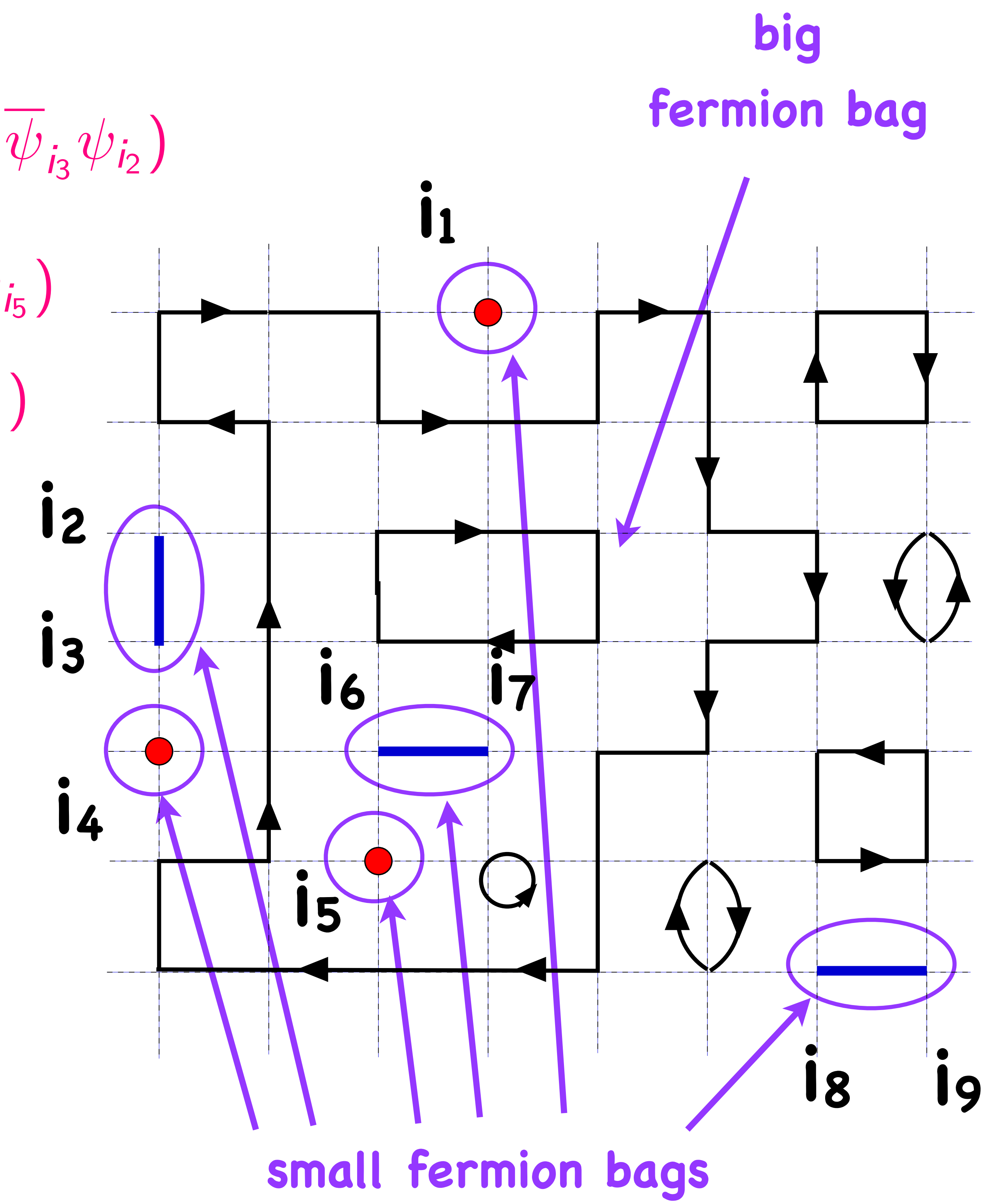
W is the matrix obtained by dropping some rows and the same columns from M



$$
M = \left(\begin{array}{ccccc|ccccc}
0 & 0 & 0 & \ldots & 0 & M_{11} & M_{12} & M_{13} & \ldots & M_{1N} \\
0 & 0 & 0 & \ldots & 0 & M_{21} & M_{22} & M_{23} & \ldots & M_{2N} \\
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. & . & . & \ldots & . & . & . & . & \ldots & . \\
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. & . & . & \ldots & . & . & . & . & \ldots & . \\
0 & 0 & 0 & \ldots & 0 & M_{N1} & M_{N2} & M_{N3} & \ldots & M_{NN} \\
\hline
-M^*_{11} & -M^*_{21} & -M^*_{31} & \ldots & -M^*_{N1} & 0 & 0 & 0\ldots & 0 & \\
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\end{array}\right)
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solvable form

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Consider actions of the form

$$S = \sum_{xy} \overline{\psi}_x \; M_{xy}[\sigma] \; \psi_x \; + \; g \sum_x \phi_x \overline{\psi}_x \psi_x \; + \; S_b(\sigma, \phi)$$

solvable

complex
scalar field

space dependent
mass term

A new class of “solvable” problems

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$$S = \sum_{xy} \overline{\psi}_x \; \underbrace{M_{xy}[\sigma]}_{\text{solvable}} \; \psi_x \; + \; g \sum_x \underbrace{\phi_x}_{\text{complex scalar field}} \underbrace{\overline{\psi}_x \psi_x}_{\text{space dependent mass term}} \; + \; S_b(\sigma, \phi)$$

The action $S_b[\sigma, \phi]$ is chosen such that

the sign problem in the k-pt correlation function

$$G(z_1, .., z_k, \sigma) \; = \; \int [d\phi] \, \mathrm{e}^{-S_b(\sigma,\phi)} \; \phi_{z_1} \; \phi_{z_2} \; ... \; \phi_{z_k}$$

is solvable.

Solvable bosonic theories are those in which we can write

$$G(z_1, .., z_k, \sigma) \ = \ \sum_b \int [d\rho] \ \ \Omega(\sigma, b, \rho, n),$$

$$\Omega(\sigma, b, \rho, n) \geq 0$$

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Dual variables (Kloiber's Talk)

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$$M[\sigma] + g\Phi \;=\; \begin{pmatrix} g\ \phi_1 & D[\sigma] \\ -D^\dagger[\sigma] & g\ \phi_2^* \end{pmatrix}$$

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suffers from sign problem

The Fermion bag approach solves the sign problem!

Fermion Bag approach

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Rewrite the partition function as

$$Z = \int [d\sigma\ d\phi]\ \mathrm{e}^{-S_b(\sigma,\phi)}\ \int [d\overline{\psi} d\psi]\ \mathrm{e}^{-\overline{\psi}\ M[\sigma]\ \psi} \prod_x \left(\mathrm{e}^{-g\ \phi_x\ \overline{\psi}_x \psi_x}\right)$$

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Due to the Grassmann nature

$$\mathrm{e}^{-g\ \phi_x\ \overline{\psi}_x \psi_x} = 1 + g\ \phi_x(-\overline{\psi}_x \psi_x) = \sum_{n_x=0,1} \left(g\ \phi_x\ (-\overline{\psi}_x \psi_x) \right)^{n_x}$$

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We can then rewrite

$$Z = \sum_{[n]} \int [d\sigma] \int [d\phi]\ \mathrm{e}^{-S_b(\sigma,\phi)} \int [d\overline{\psi} d\psi]\ \mathrm{e}^{-\overline{\psi}\ M\ \psi} \prod_x \left(g\ \phi_x\ (-\overline{\psi}_x \psi_x)\right)^{n_x}$$

Consider a configuration [n]
where z_1 z_2 ... z_k are the k sites
where $n_x = 1$
and all other sites have $n_x = 0$

example of configuration [n] with k = 10

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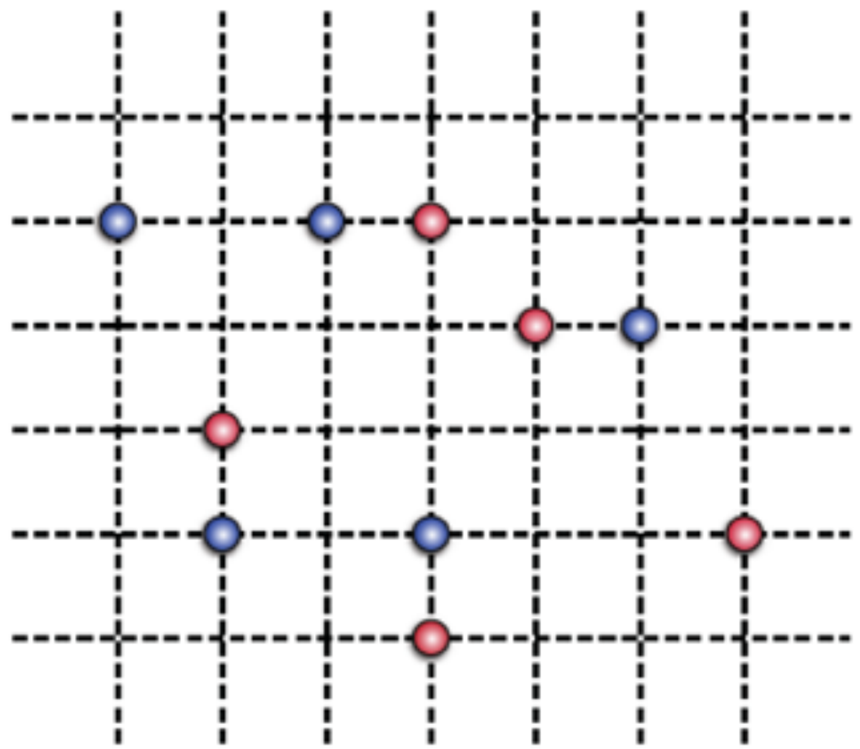

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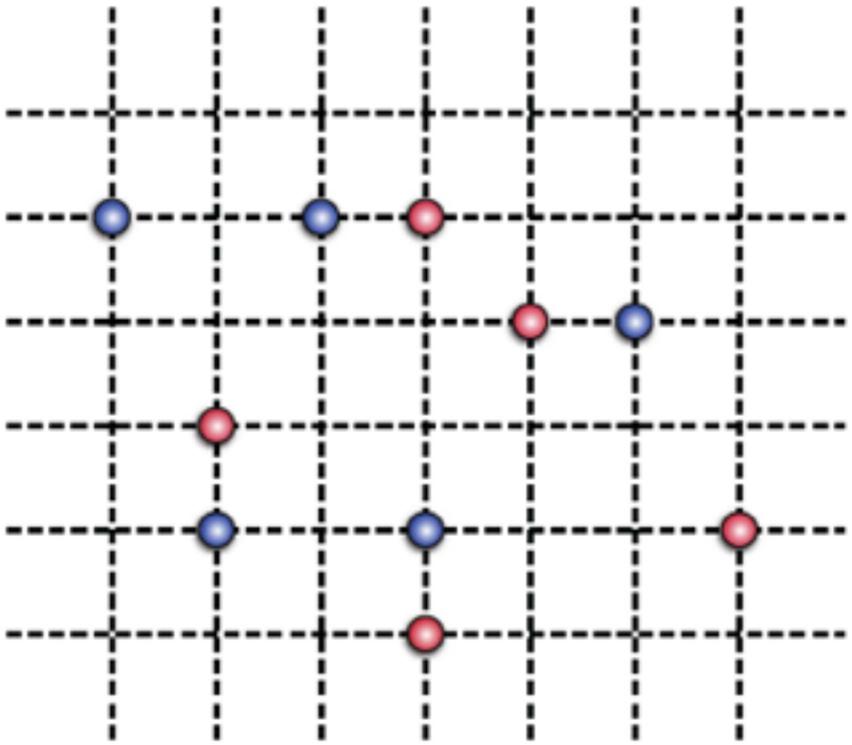
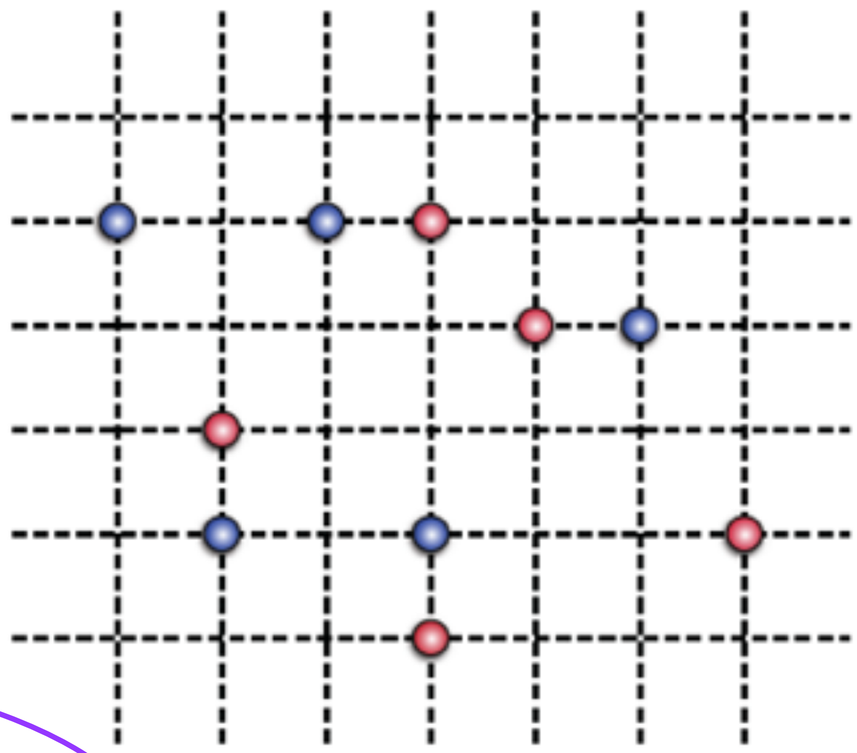


$$Z = \sum_{[n]} g^k \int [d\sigma] \int [d\phi]\, \mathrm{e}^{-S_b(\sigma,\phi)}\, \phi_{z_1}\, \phi_{z_2}\, \ldots\, \phi_{z_k}$$

$$\int [d\overline{\psi} d\psi]\, \mathrm{e}^{-\overline{\psi}\, M[\sigma]\, \psi}\, (-\overline{\psi}_{z_1}\psi_{z_1})\, (-\overline{\psi}_{z_2}\psi_{z_2})\, \ldots\, (-\overline{\psi}_{z_k}\psi_{z_k})$$

example of configuration [n] with k = 10



Consider a configuration [n] where z_1 z_2 ... z_k are the k sites where $n_x = 1$ and all other sites have $n_x = 0$

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$$G(z_1, .., z_k, \sigma)$$

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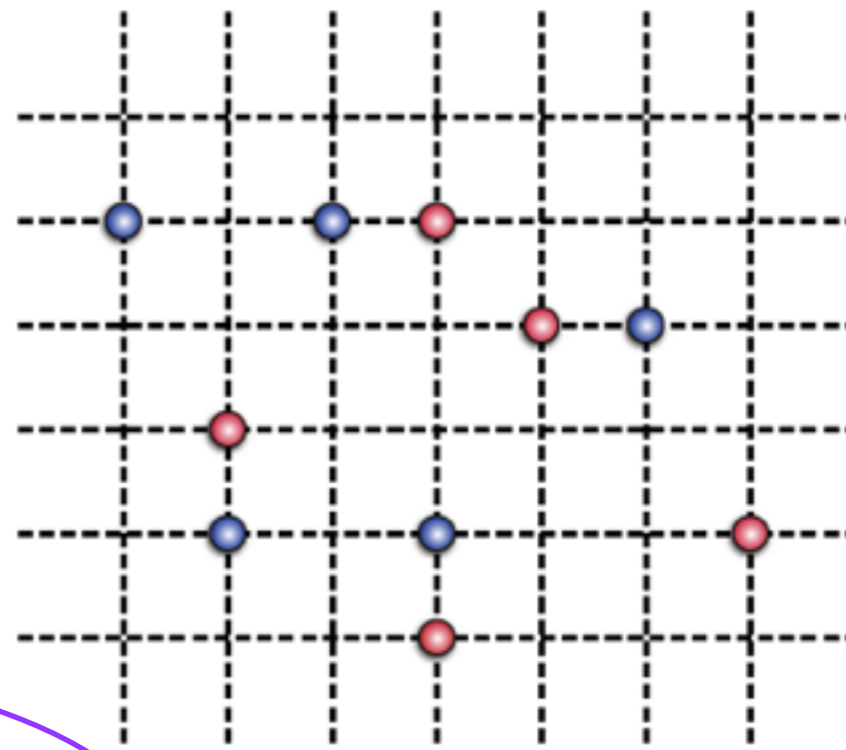

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Fermion Correlation Function

Fermion correlation function

$$\int [d\overline{\psi} d\psi] \; \mathrm{e}^{-\overline{\psi} \; M[\sigma] \; \psi} \; \overline{\psi}_{z_1} \psi_{z_1} \; ... \; \overline{\psi}_{z_k} \psi_{z_k}$$

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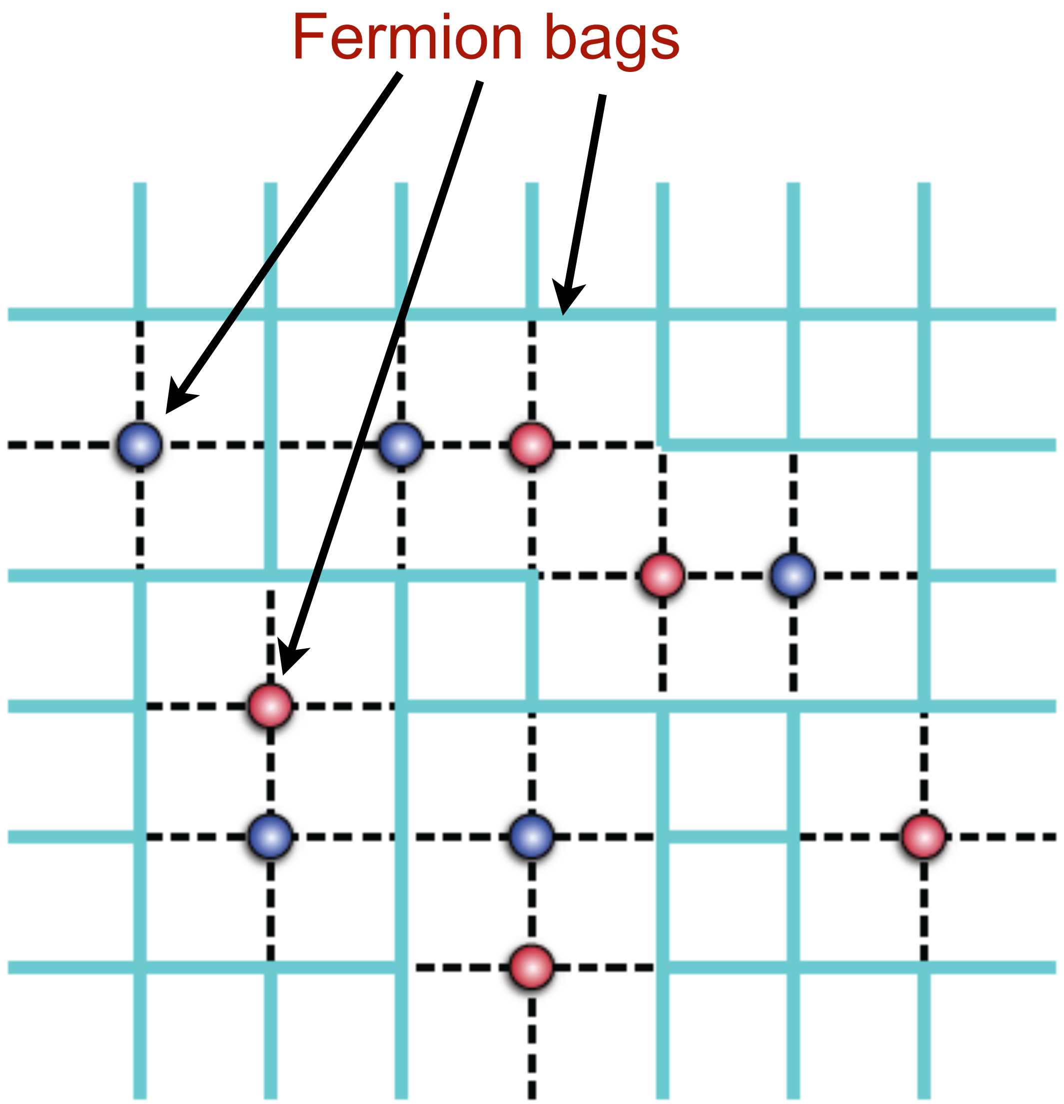

fermion bag configuration

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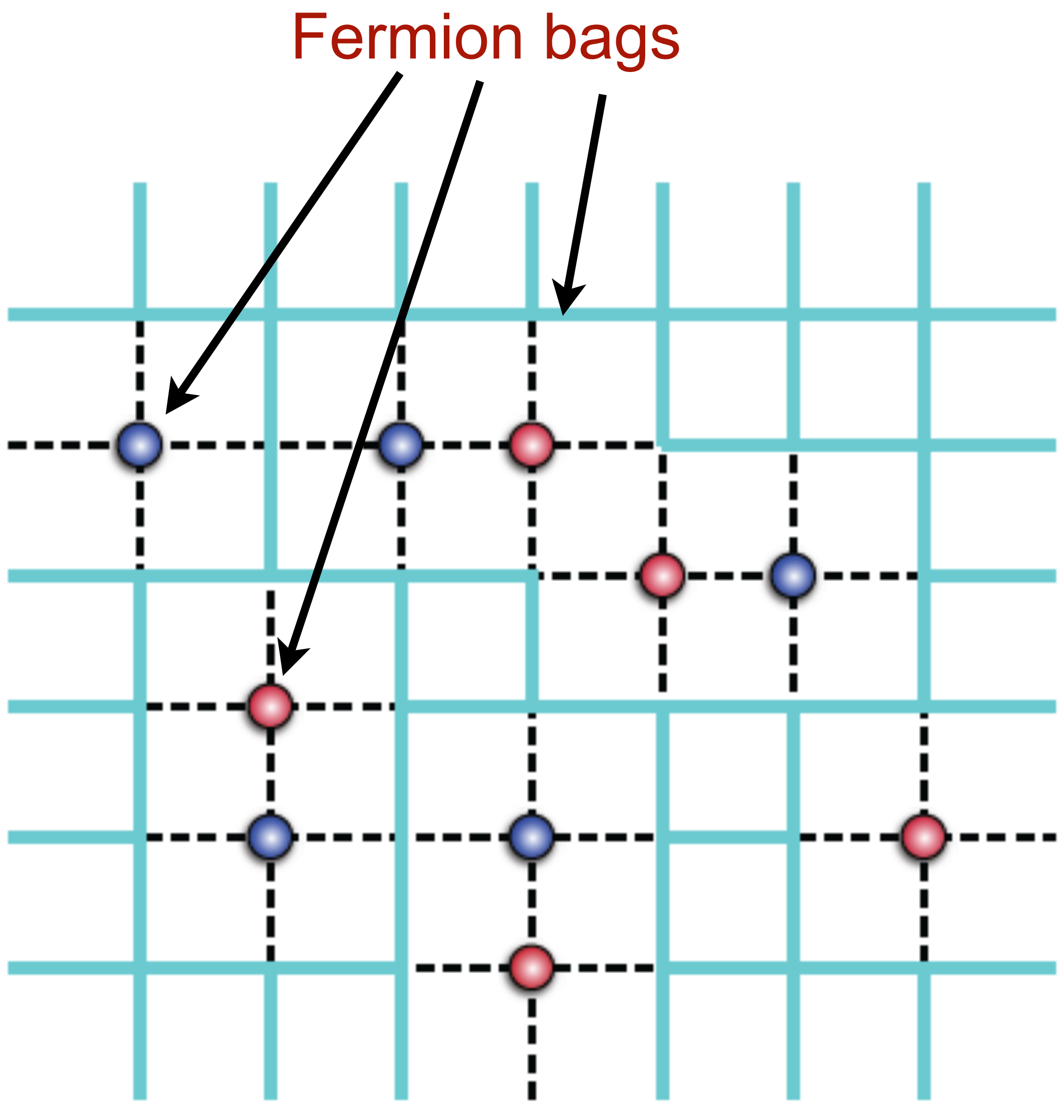
$$=\ \mathrm{Det}(W[n,\sigma]) \geq 0$$



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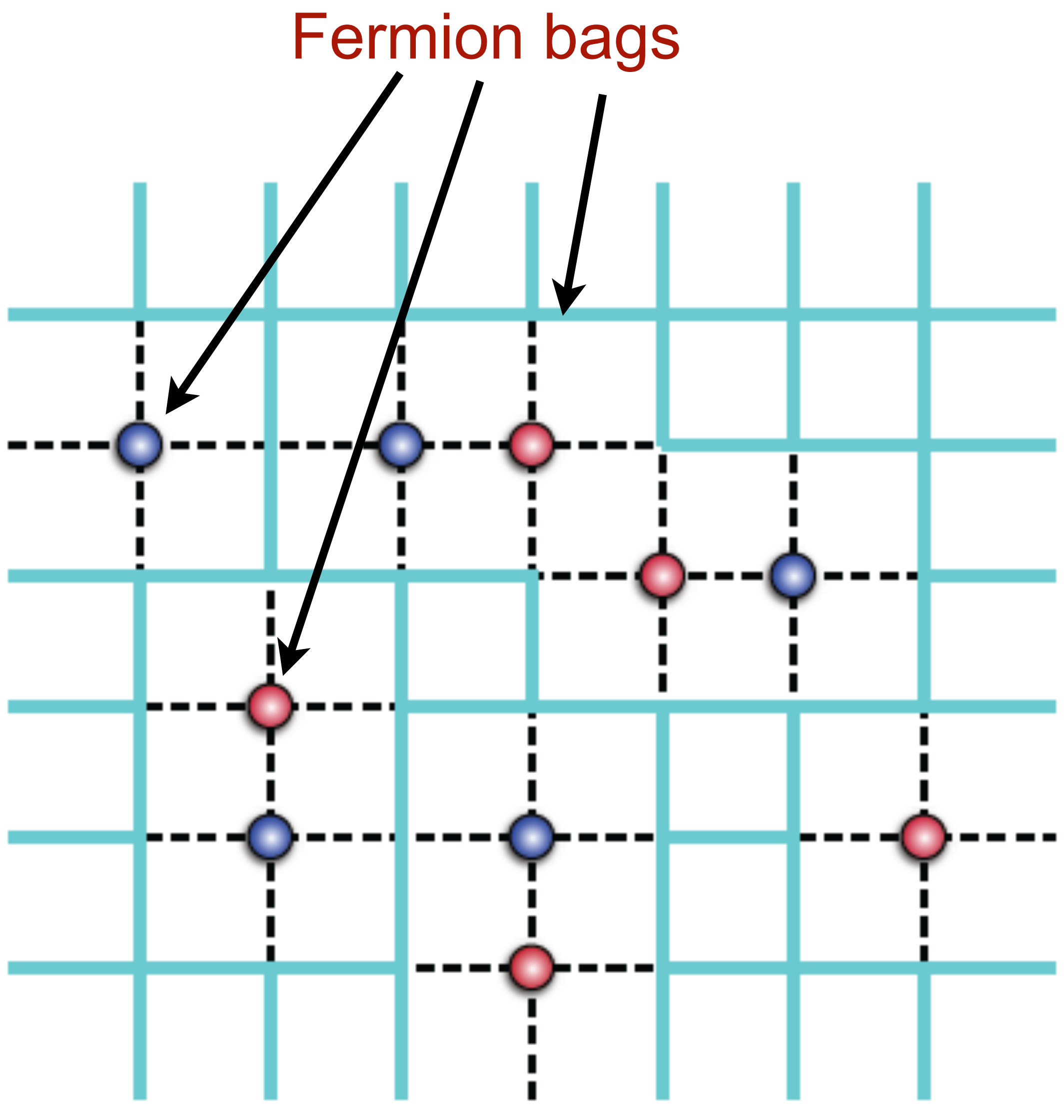

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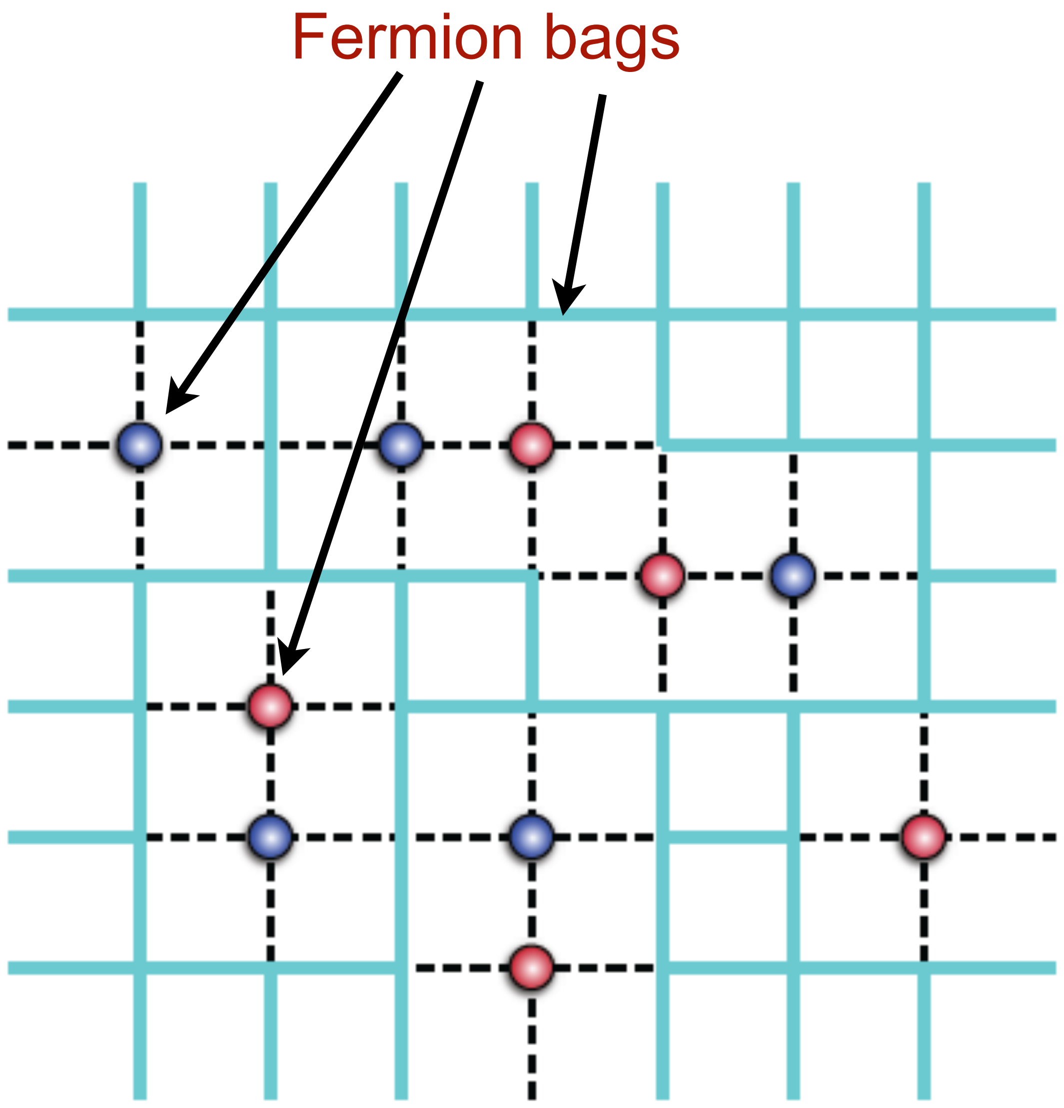

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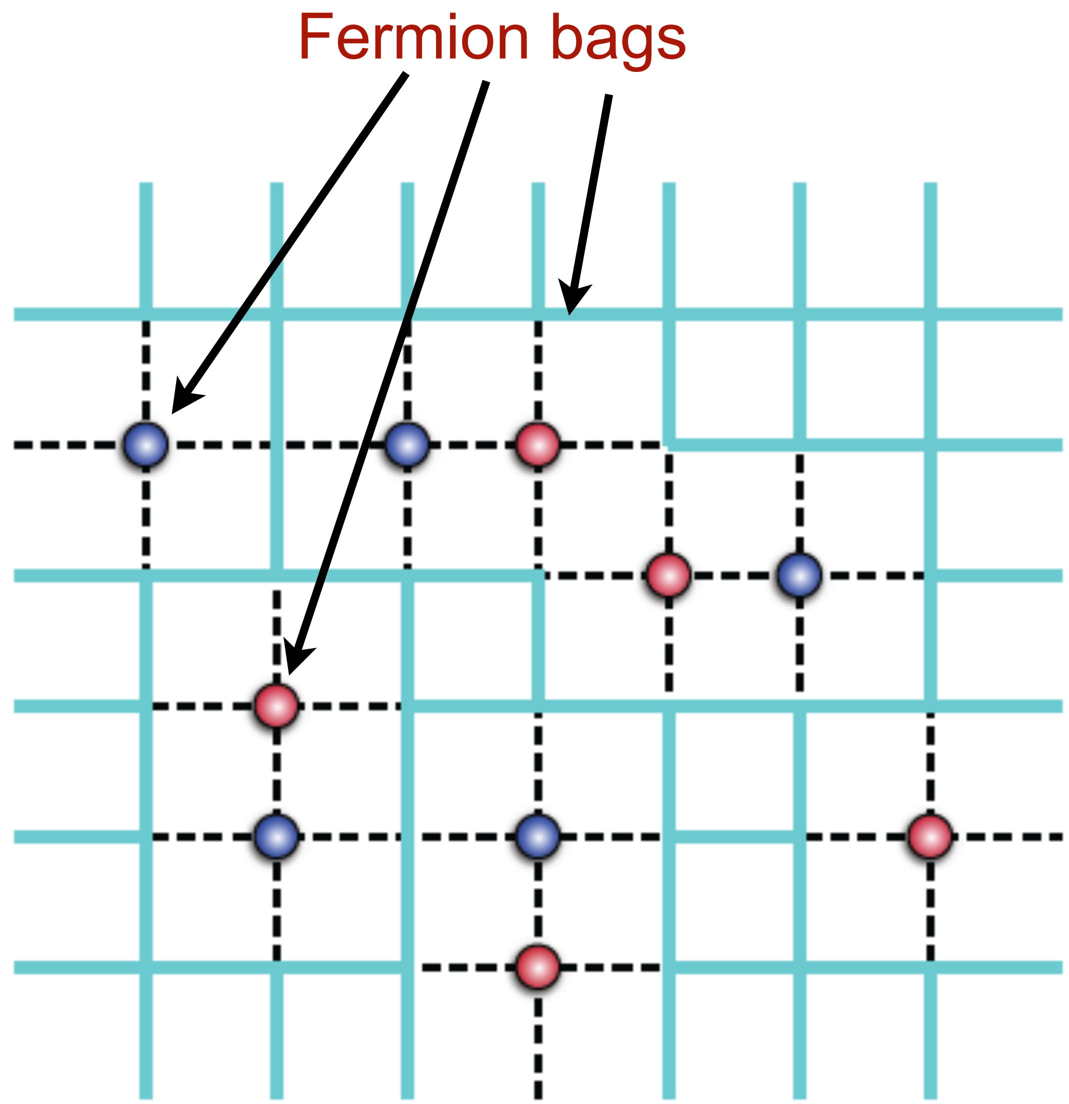

fermion bag configuration

Connection to Diagrammatic Determinantal MC
Talks by Endres and Detmold

Thus, the partition function
is given by

$$Z = \sum_{n,b} \int [d\sigma \; d\rho] \;\; g^k \; \Omega(\sigma, b, \rho, n) \; \mathrm{Det}(W[n,\sigma])$$

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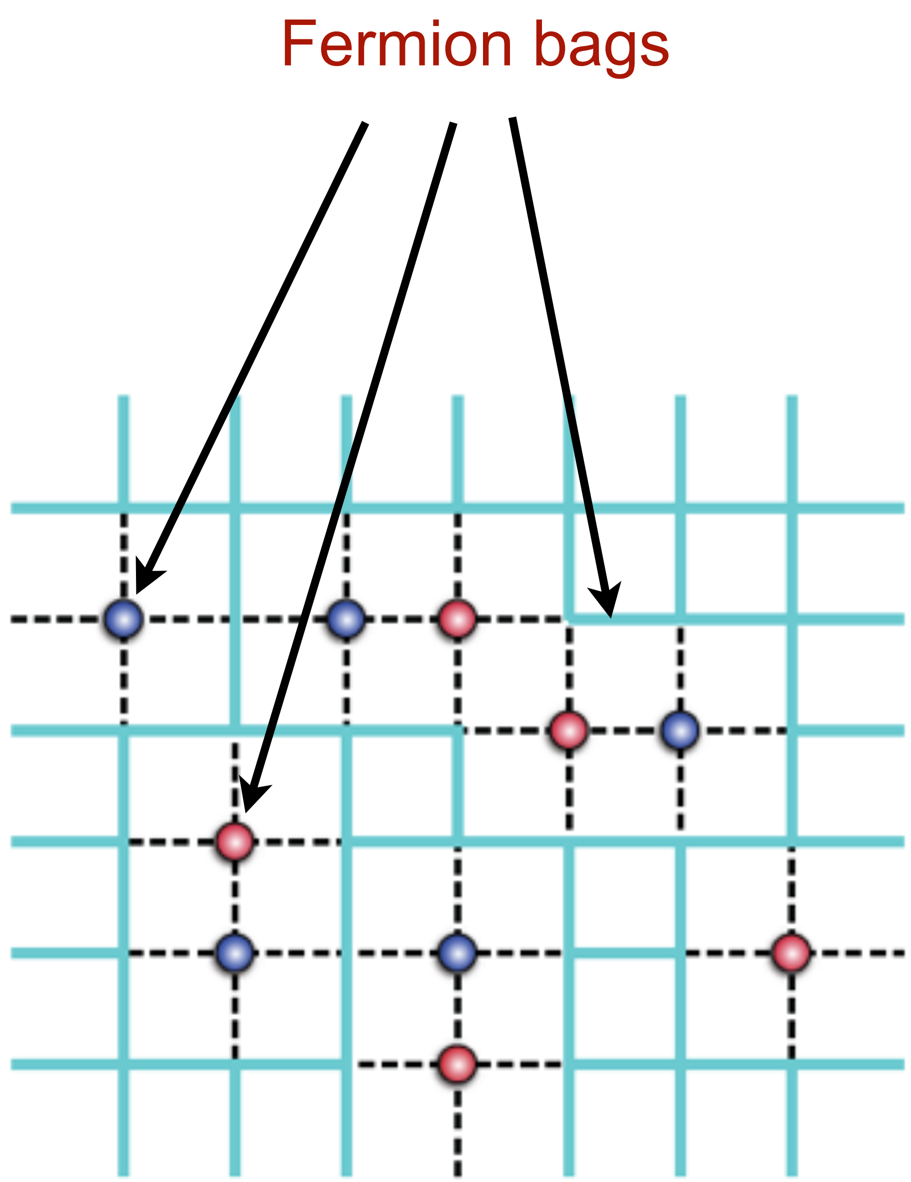

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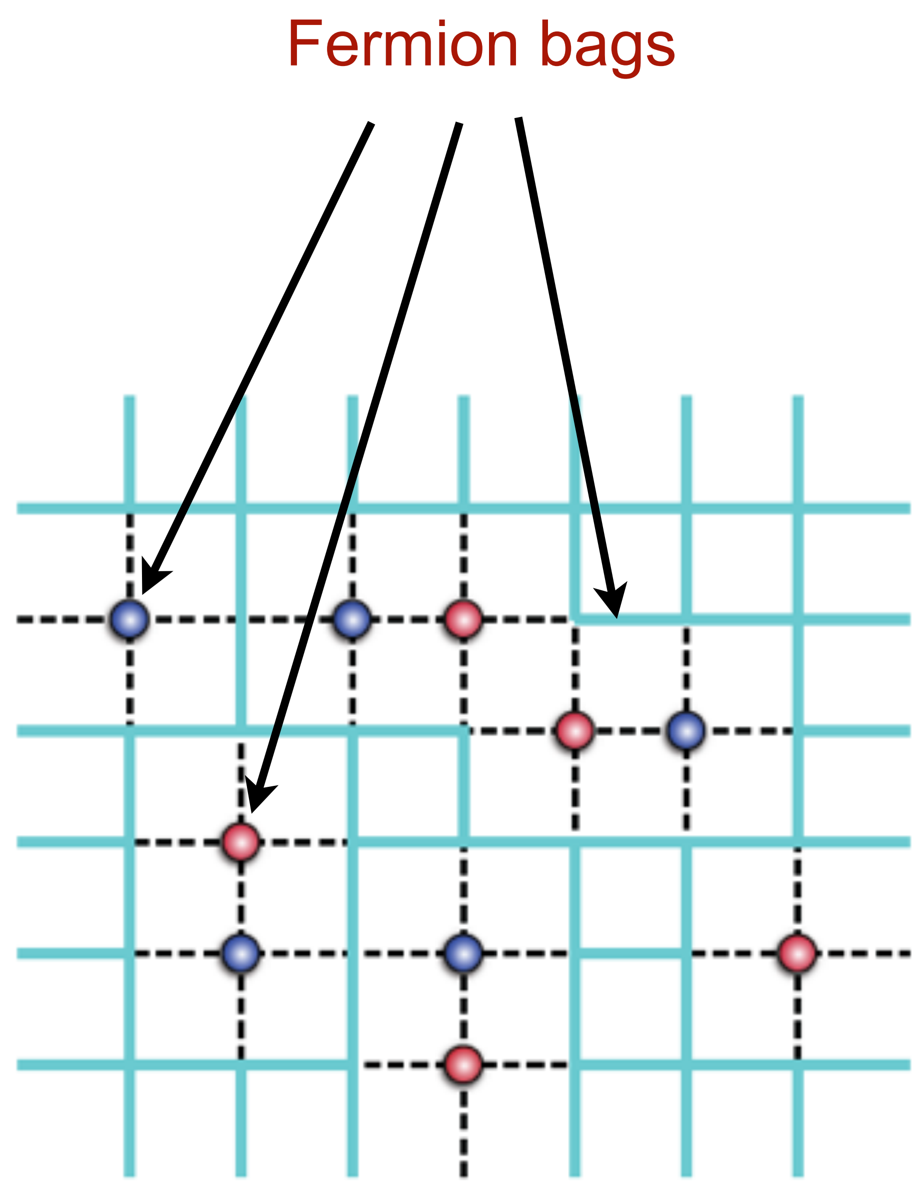
No sign problem!



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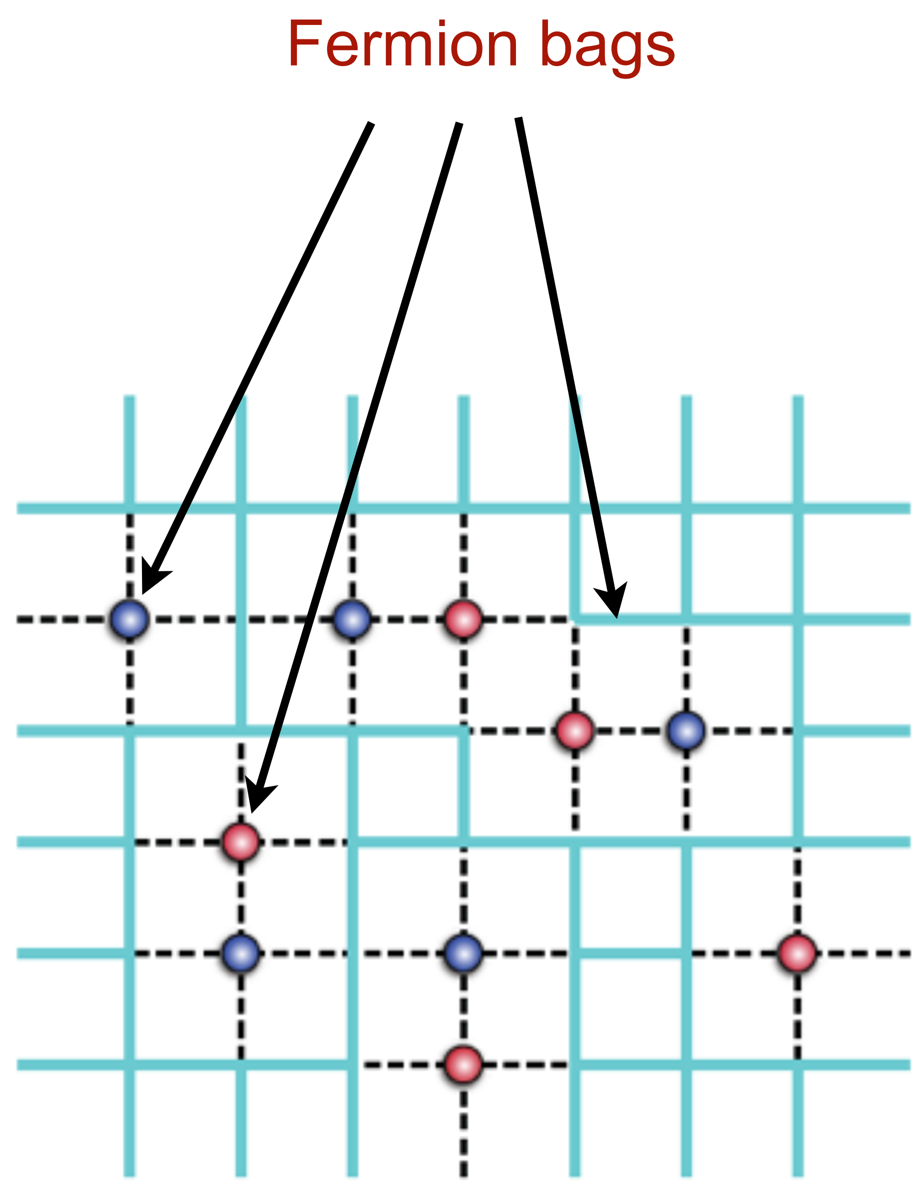
Interesting mapping into classical statistical mechanics



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Another class of “solvable” problems

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Consider actions of the form

$$S = \sum_{xy} \overline{\psi}_x \; M_{xy}[\sigma] \; \psi_x - i \sum_x \; \left(\; g_1 \phi_{1x} \psi_x^T \sigma_2 \psi_x - g_2 \; \phi_{2x} \overline{\psi}_x \sigma_2 \overline{\psi}_x^T \right) + S_b(\sigma, \phi_1, \phi_2)$$

where $\psi_x, \; \overline{\psi}_x$ are two component Grassmann fields

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Such problems naturally describe "pairing" of fermions like in a superconductor

$$
M = \left(\begin{array}{ccccc|ccccc}
C_{11} & C_{12} & C_{13} & \dots & C_{1N} & M_{11} & M_{12} & M_{13} & \dots & M_{1N} \\
C_{21} & C_{22} & C_{23} & \dots & C_{2N} & M_{21} & M_{22} & M_{23} & \dots & M_{2N} \\
C_{31} & C_{32} & C_{33} & \dots & C_{3N} & M_{31} & M_{32} & M_{33} & \dots & M_{3N} \\
. & . & . & \dots & . & . & . & . & \dots & . \\
. & . & . & \dots & . & . & . & . & \dots & . \\
. & . & . & \dots & . & . & . & . & \dots & . \\
C_{N1} & C_{N2} & C_{N3} & \dots & C_{NN} & M_{N1} & M_{N2} & M_{N3} & \dots & M_{NN} \\
\hline
-M^*_{11} & -M^*_{12} & -M^*_{13} & \dots & -M^*_{1N} & C^*_{11} & C^*_{12} & C^*_{13} & \dots & C^*_{1N} \\
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. & . & . & \dots & . & . & . & . & \dots & . \\
. & . & . & \dots & . & . & . & . & \dots & . \\
. & . & . & \dots & . & . & . & . & \dots & . \\
-M^*_{1N} & -M^*_{2N} & -M^*_{3N} & \dots & -M^*_{NN} & C^*_{N1} & C^*_{N2} & C^*_{N3} & \dots & C^*_{NN}
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$$

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solvable form

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Challenge: Understand “solvability” with non-Abelian fields

Dual Variables(?)
Subset methods, Bloch’s Talk

A QCD-like Polyakov-Loop Model may be “solvable”(?)

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Action $$S = \sum_{xy} \overline{\psi}_x M_{xy}[z, z^*, \mu]\psi_y + S_b(z)$$

massless staggered Dirac operator

Z_3 Polyakov-Loop variables

Z_3 Potts Model

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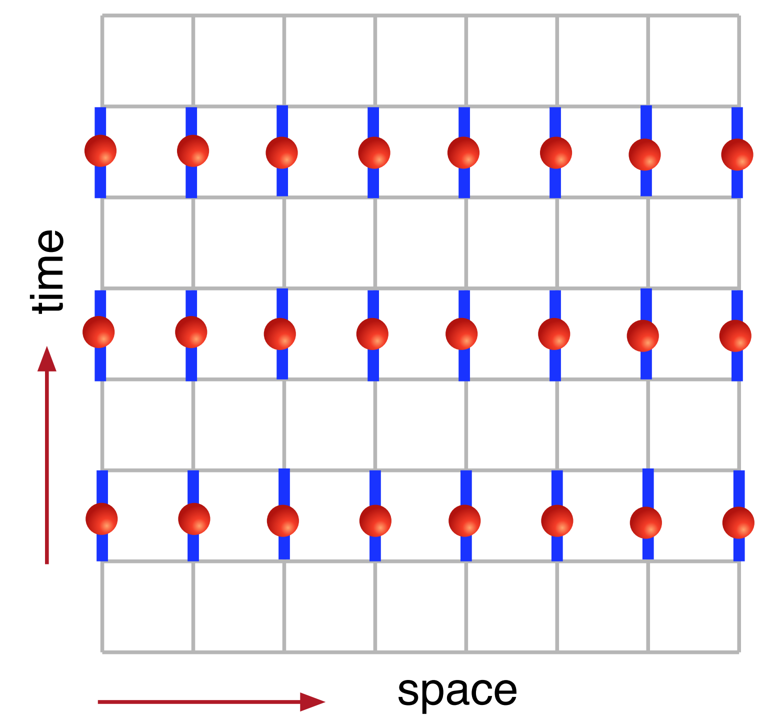
Z_3 Potts Model

Constraint:
The Polyakov-Loop variables live only on alternate time slices!



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$$S = \sum_{xy} \overline{\psi}_x D_{xy} \psi_x + \overline{\chi}_x D_{xy} \chi_x$$

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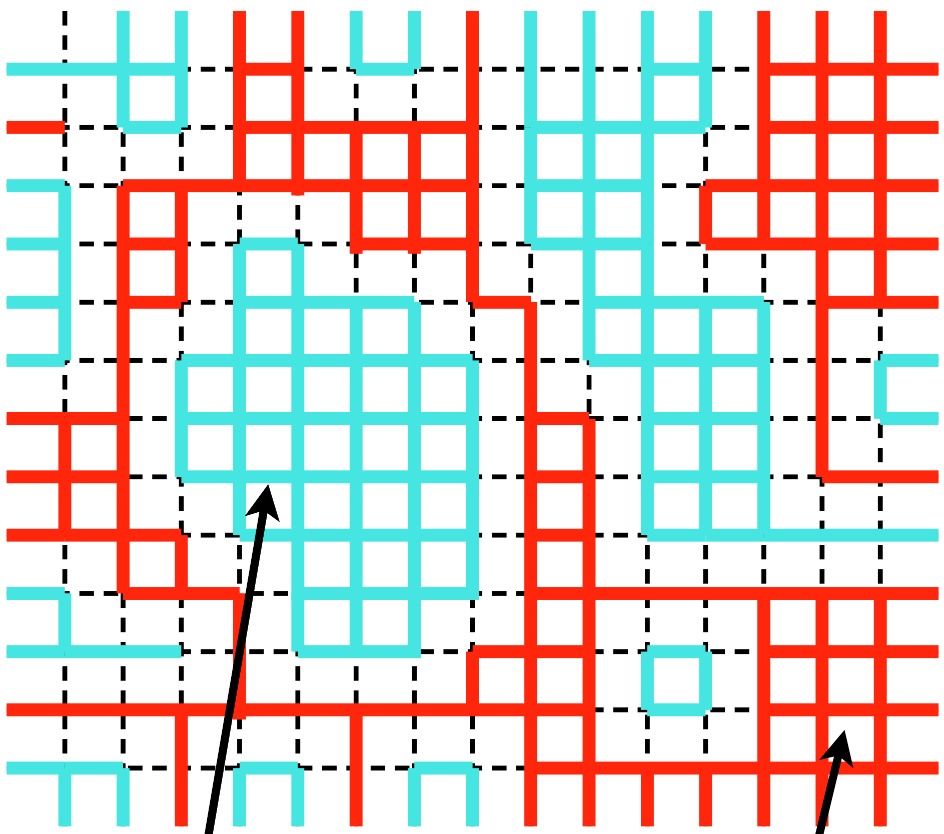
Fermion Bag Configuration



fermion bag containing species 1

fermion bag containing species 2

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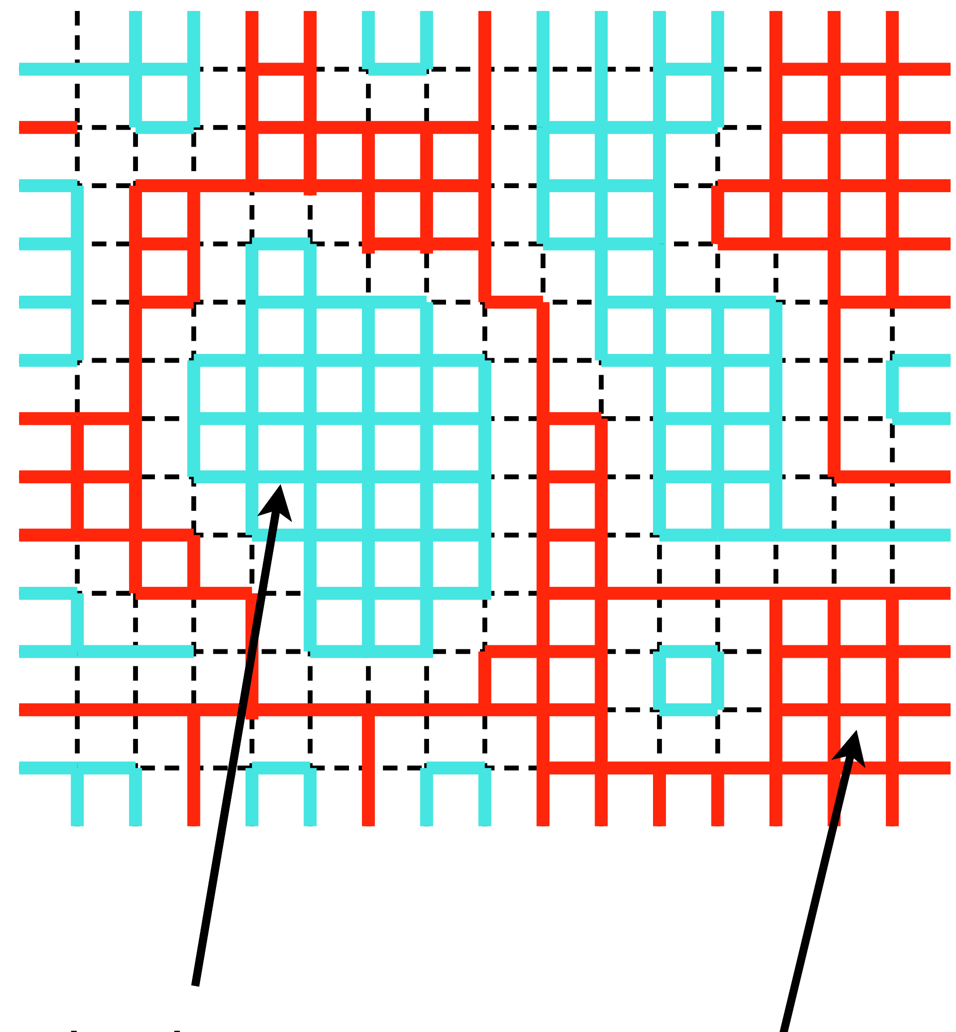
repulsion

$$Z = \sum_{B} |\mathrm{Det}(W_A)|^2 \; |\mathrm{Det}(W_B)|^2$$

Fermion Bag Configuration



fermion bag
containing species 1

fermion bag
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Some repulsive models also solvable!

$$S = \sum_{xy} \overline{\psi}_x D_{xy} \psi_x + \overline{\chi}_x D_{xy} \chi_x$$

$$- \sum_x \left\{ U(\overline{\psi}_x \psi_x)^2 + U(\overline{\chi}_x \chi_x)^2 - U^2 (\overline{\psi}_x \psi_x)^2 (\overline{\chi}_x \chi_x)^2 \right\}$$

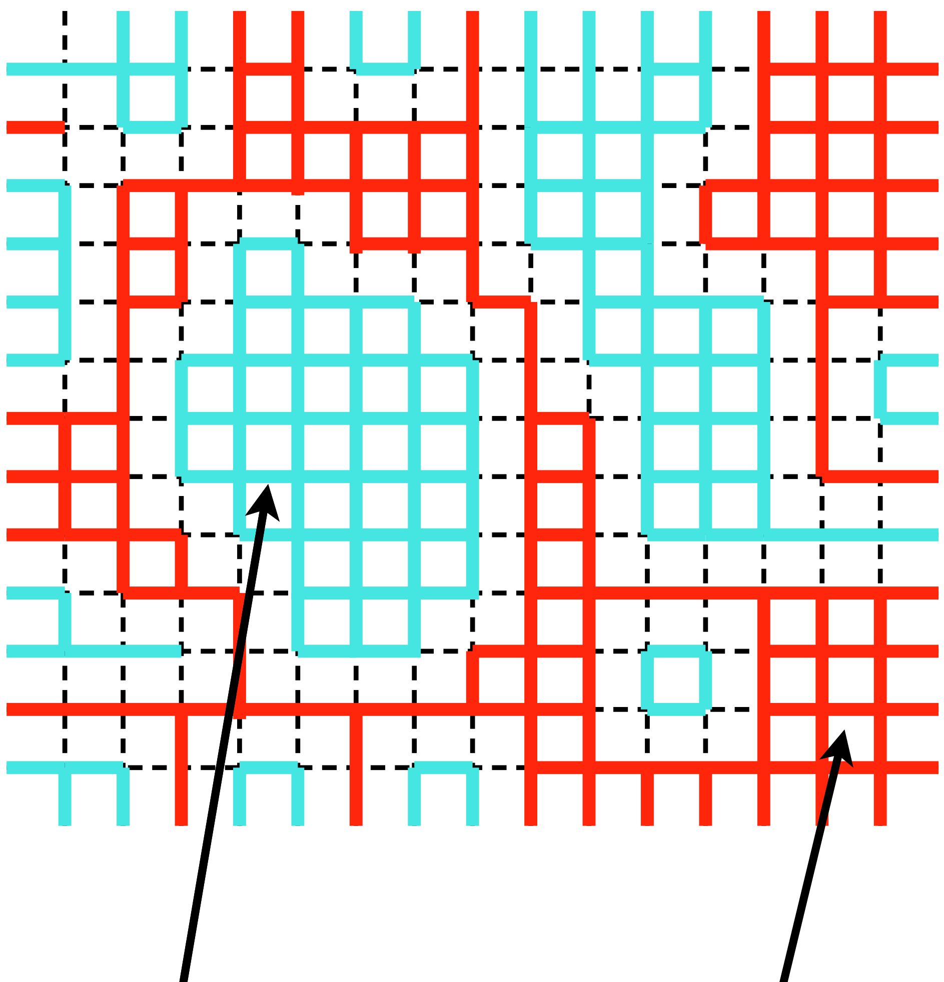
attractive

repulsion

$$Z = \sum_B |\mathrm{Det}(W_A)|^2 \; |\mathrm{Det}(W_B)|^2$$

No sign problem!

Fermion Bag Configuration



MC Results: Four-Fermion Models

S.C. A.Li, PRL (2012), arXiv:1304.7761

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SU(2) x U(1) symmetric models

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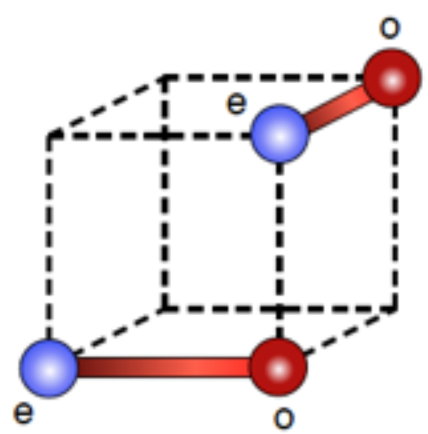

Thirring

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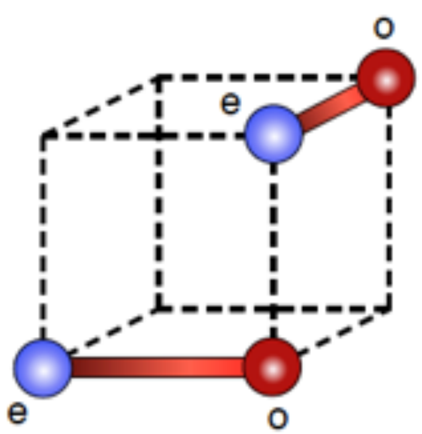

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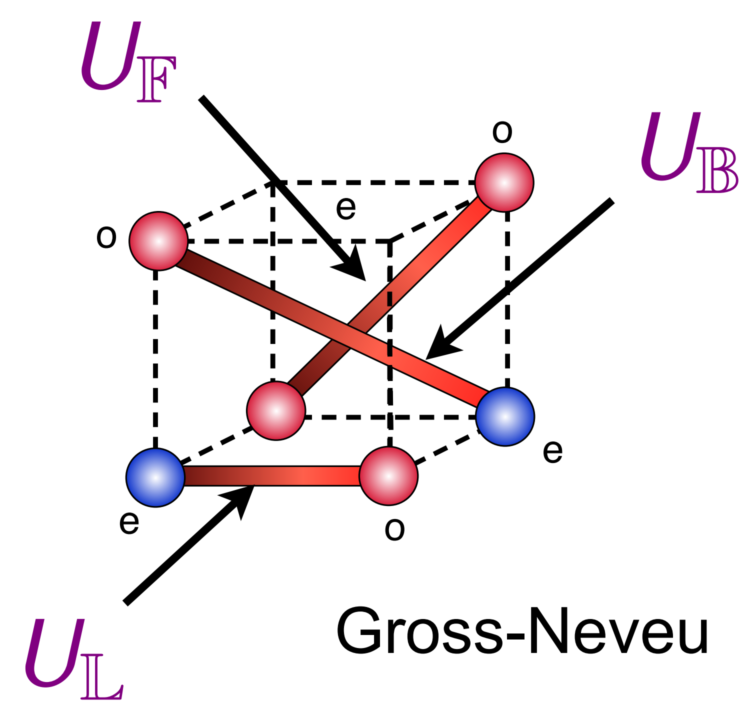

Gross-Neveu

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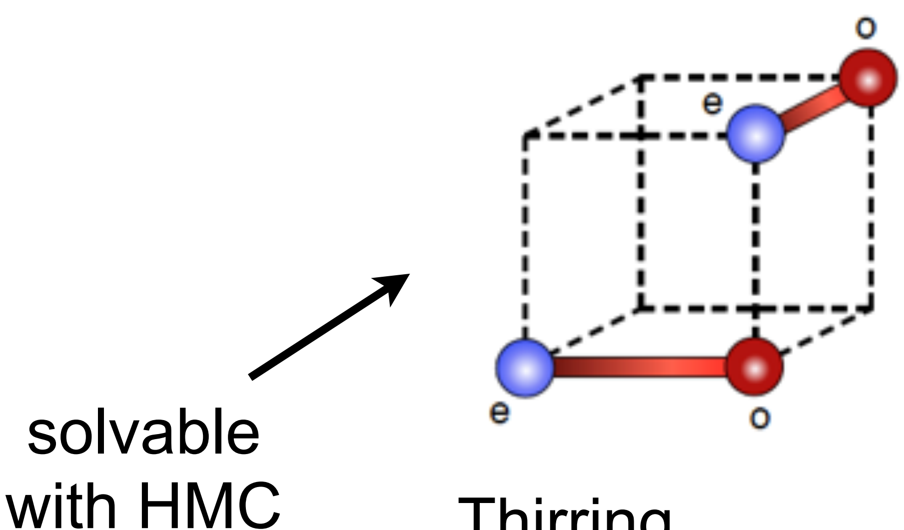

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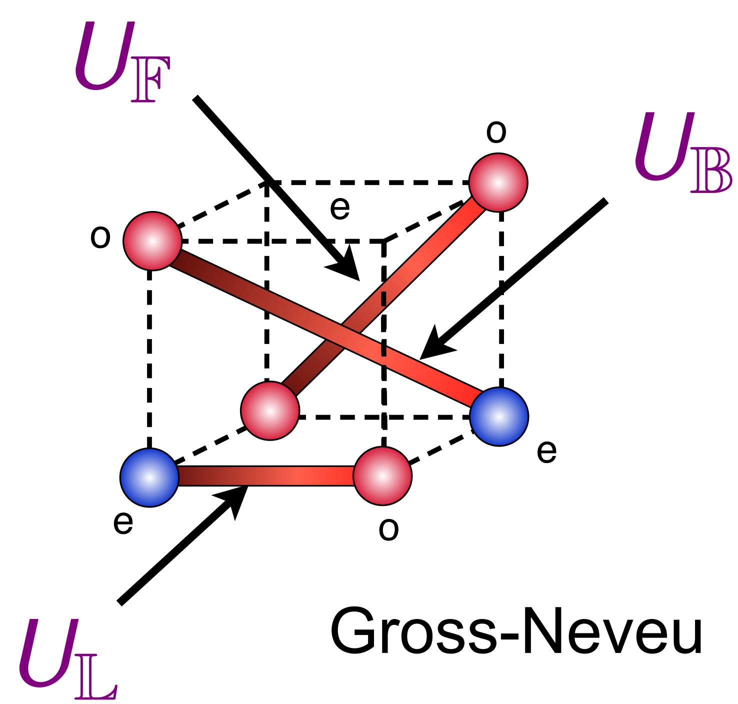

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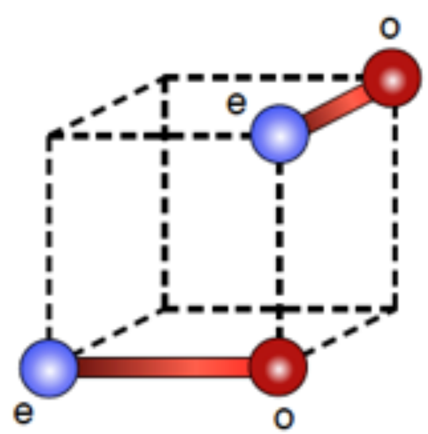
solvable with HMC



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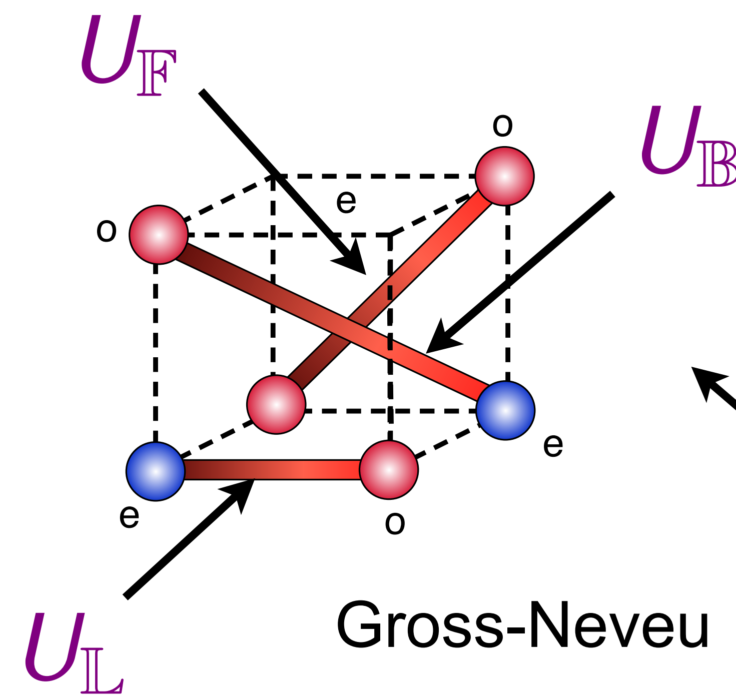

Gross-Neveu

suffers from sign problems in HMC

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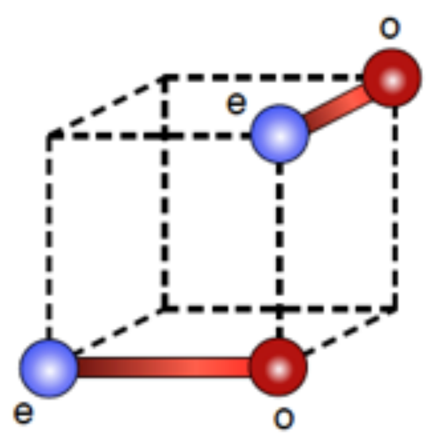

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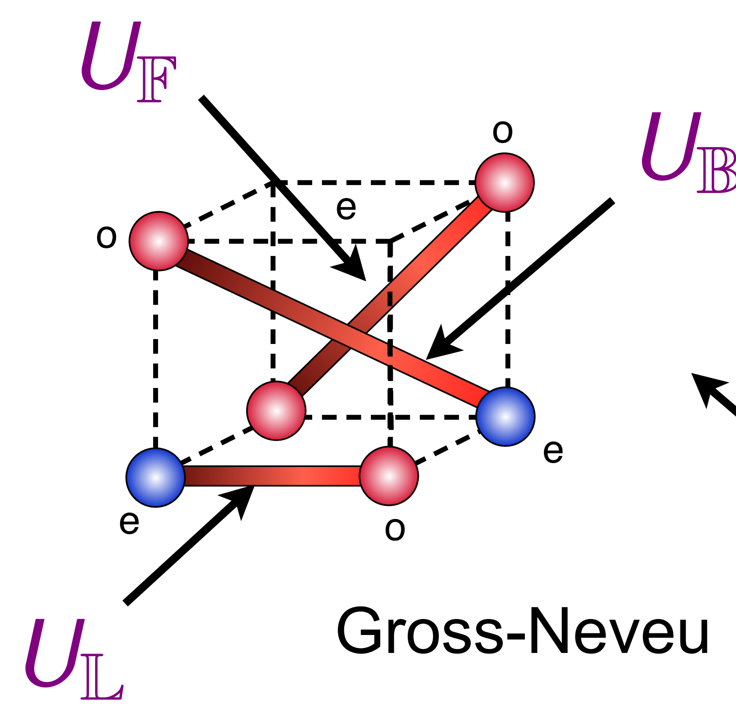
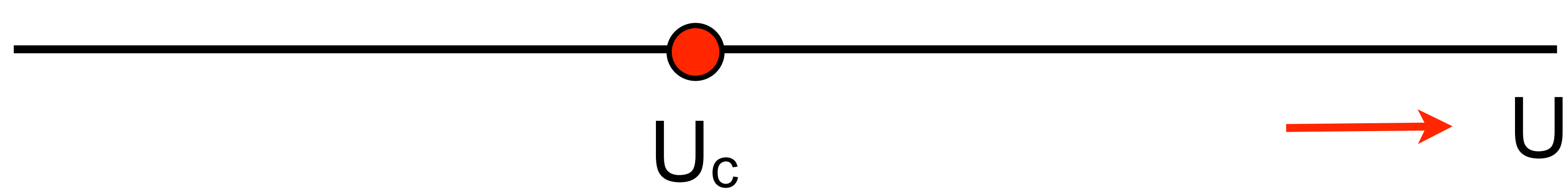


Gross-Neveu

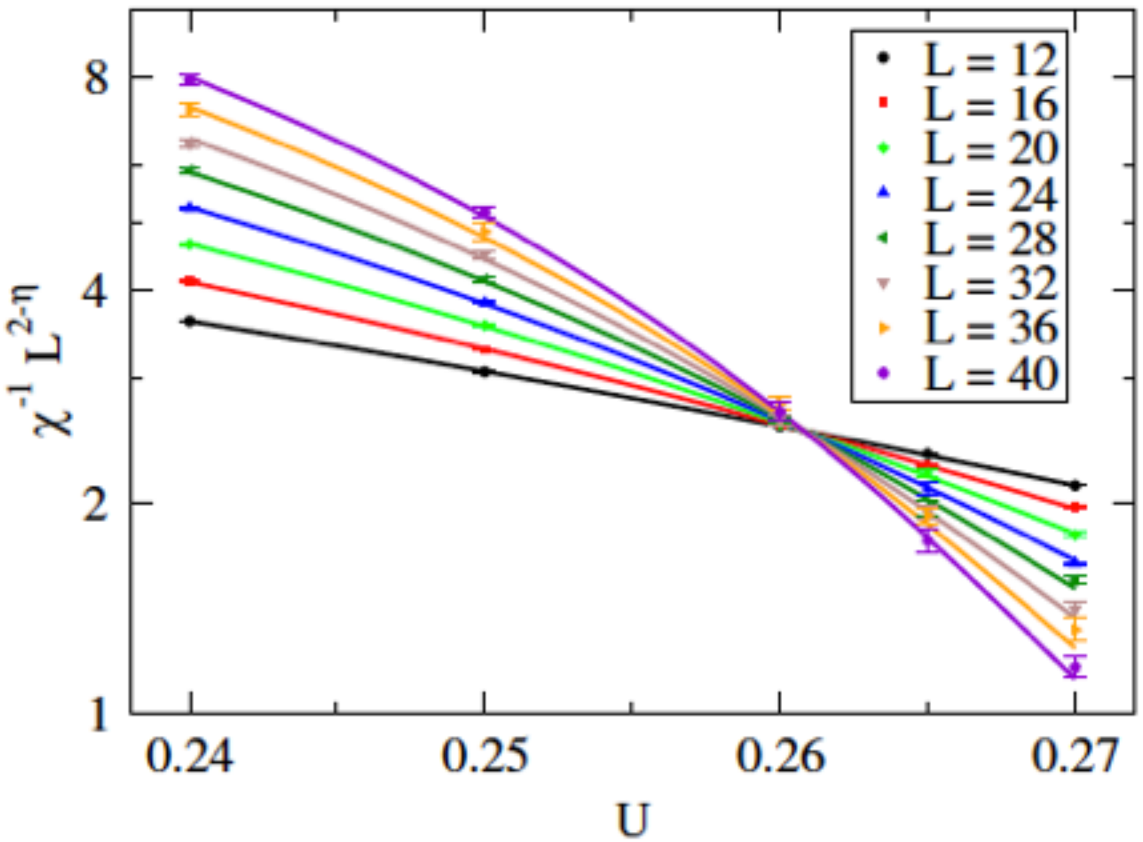
suffers from
sign problems
in HMC

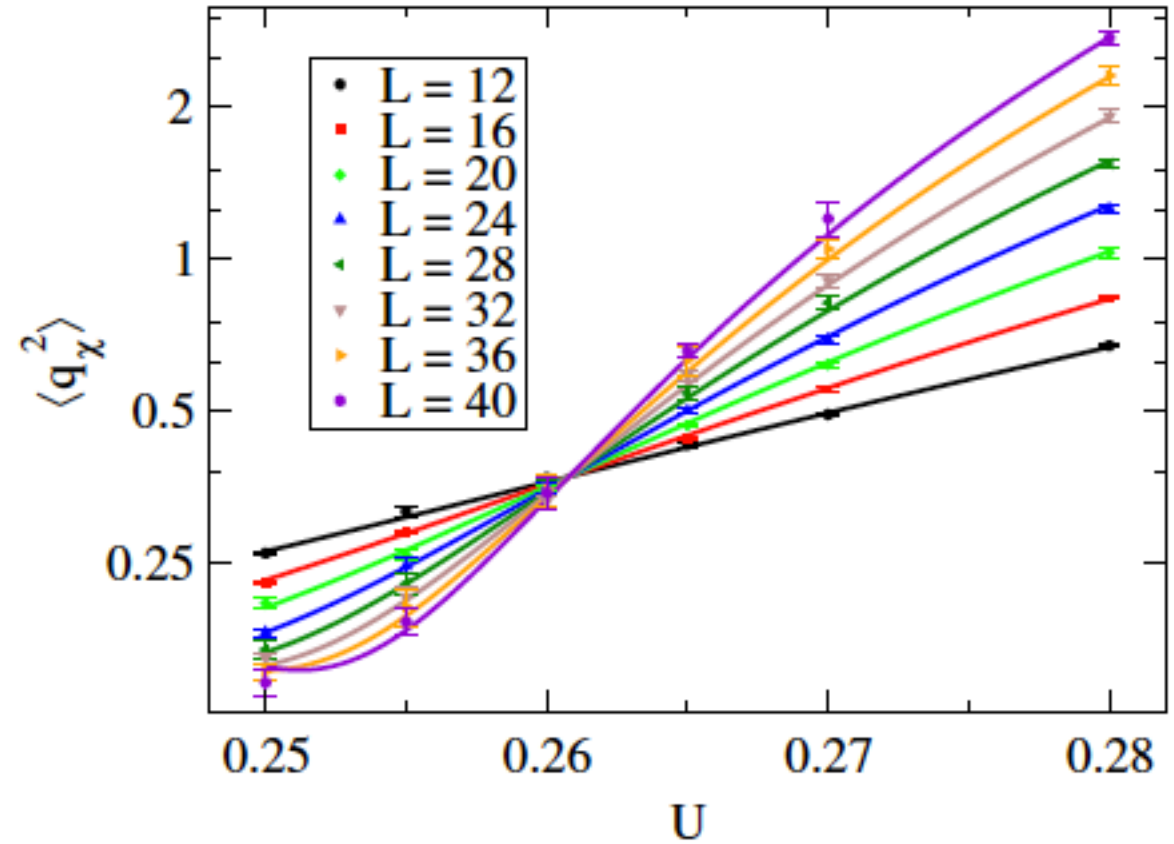
massless fermions/
U(1) symmetric

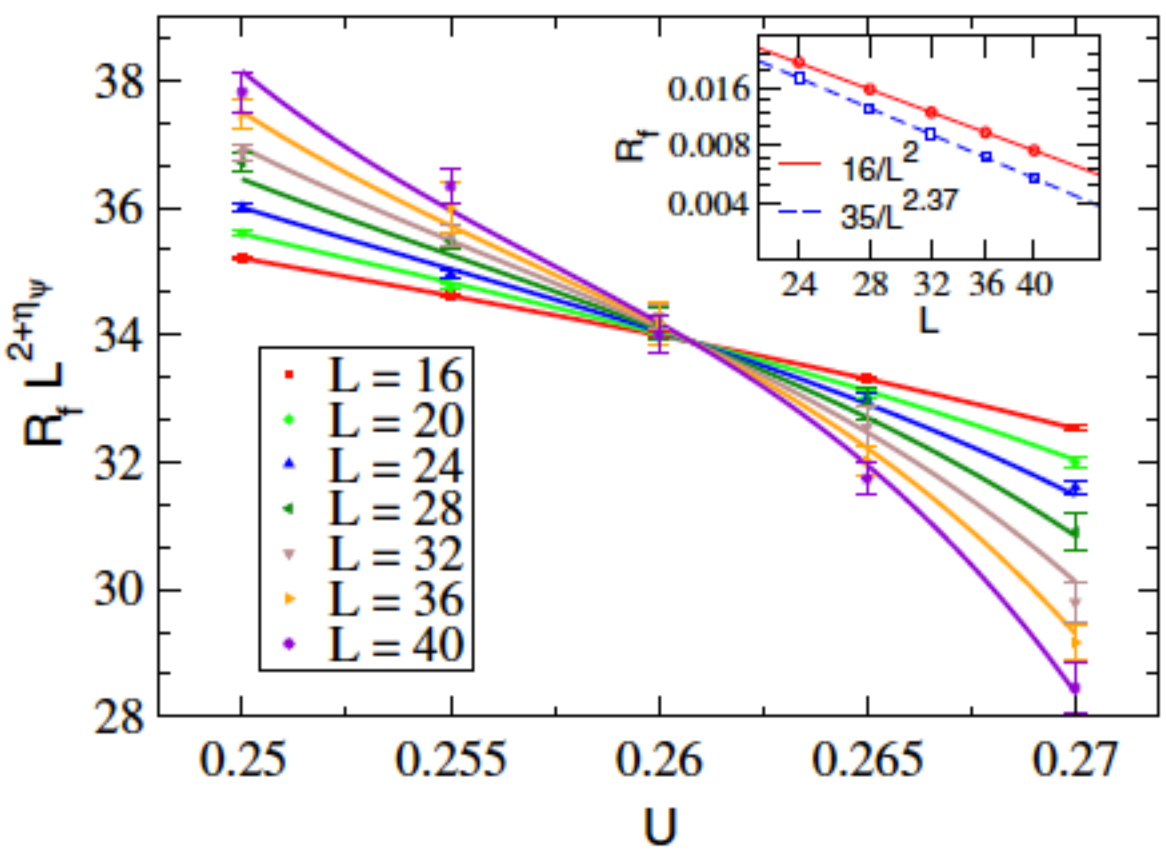
massive fermions/
U(1) broken



Thirring model results







Combined fit results

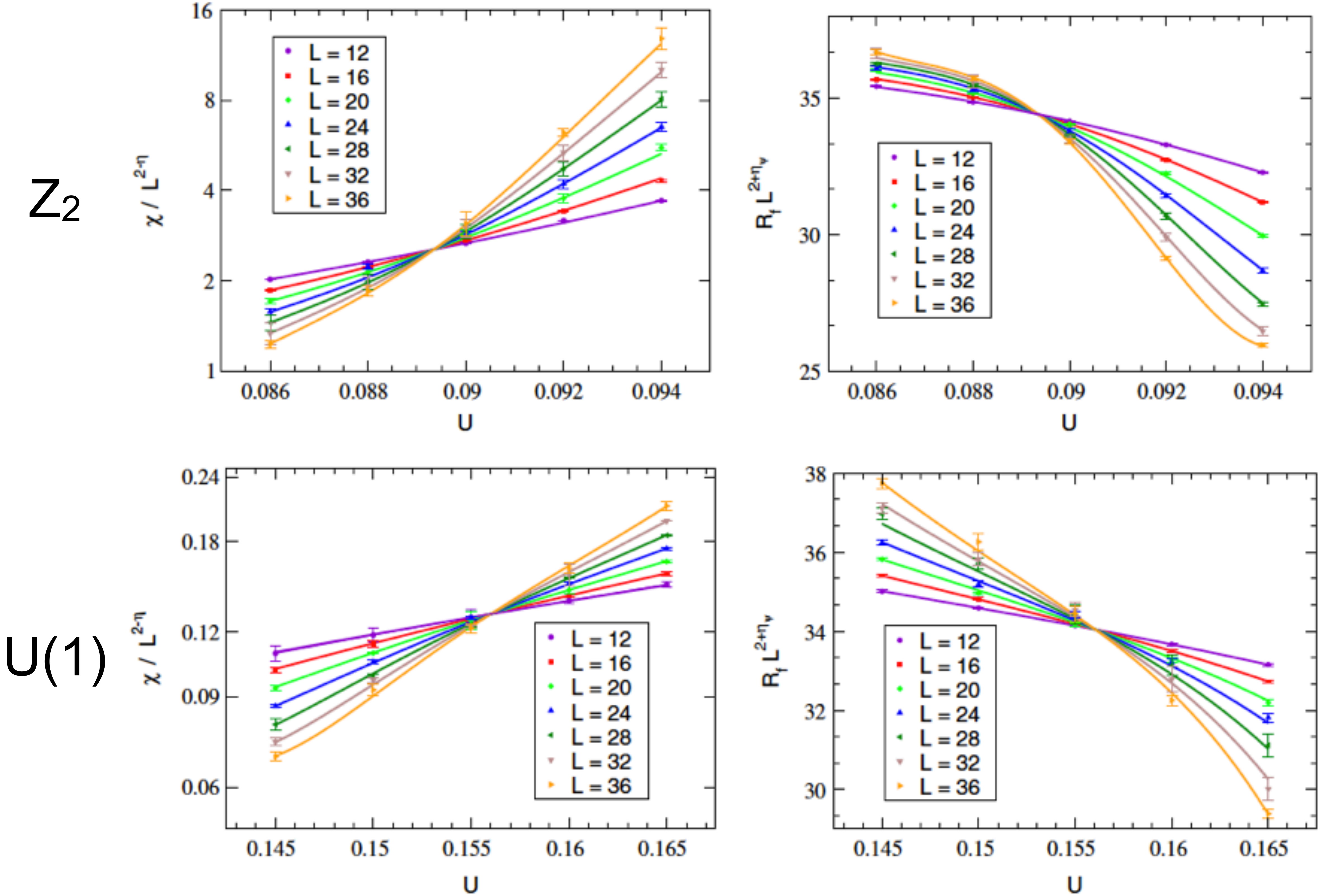
$U_c = 0.2608(2)$

$\nu = 0.85(1)$

$\eta = 0.65(1)$

$\eta_\psi = 0.37(1)$

Gross-Neveu Model Results



Comparison: Old vs New

Model	Symmetry	Work	ν	η	η_ψ
N=1 Lattice-GN	SU(2) x Z_2	Karkkainen,et.al. (1994)	1.00(4)	0.756(8)	-
N=1 Lattice GN	SU(2) x Z_2	SC & Li (2012)	0.83(1)	0.62(1)	0.38(1)
N = 1 Lattice-Th	SU(2)x U(1)	Debbio, et.al., (1997)	0.80(15)	0.70(15)	-
N = 1 Lattice-Th	SU(2)x U(1)	Barbour et. al., (1998)	0.80(20)	0.4(2)	-
N=1 Lattice-(GN/Th)	SU(2) x U(1)	SC & Li (2013)	0.849(8)	0.633(8)	0.373(3)

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- Precision Quantum Critical Behavior in a class of Fermi systems is within reach.