

Fermion Bag Approach to Fermion Sign Problems

**Shailesh Chandrasekharan
(Duke University)**

Collaborator (Anyi Li, INT)

Outline

- Review fermions in Quantum Field Theory
- A new look at Grassmann Integration and Fermion Bags
- Lessons from a Plaquette Model
- New Class of Solvable Models
- Some Recent Results
- Conclusions

Fermions in Quantum Field Theory

Partition function

$$Z = \int [d\phi] \int [d\bar{\psi} d\psi] e^{-S_b[\phi] - S_f(\bar{\psi}, \psi, \phi)}$$

Here ψ and $\bar{\psi}$ are two independent Grassmann valued fields on a lattice while ϕ is a bosonic field.

What are Grassmann variables?

Grassmann Calculus

Two Grassmann variable anticommute

$$\psi_1 \psi_2 = -\psi_2 \psi_1$$

This implies $\psi^2 = 0$

Integration rules are very simple

$$\int d\psi = 0, \quad \int d\psi \psi = 1$$

This implies

$$\int \prod_i (d\bar{\psi}_i d\psi_i) e^{-\bar{\psi}_i M_{ij} \psi_j} = \text{Det}(M)$$

Traditional Approach

Scalettar, Scalapino, Sugar, Toussaint (1986,1987)

Rewrite partition functions as

$$Z = \int [d\sigma] \int [d\bar{\psi} d\psi] e^{-S_b[\sigma] - \sum_{i,j} \bar{\psi}_i M_{ij}[\sigma] \psi_j}$$

Then integrate over the Grassmann variables

$$Z = \int [d\sigma] e^{-S_b[\sigma]} \text{Det}(M[\sigma])$$

If $\text{Det}(M[\sigma])$ is positive then sign problem is solved!

Unfortunately, determinants are NOT always positive!

Solvable problems (mostly!) are of the type

$$M[\sigma] = \begin{pmatrix} 0 & D[\sigma] \\ -D^\dagger[\sigma] & 0 \end{pmatrix}$$

“solvable form”

(in an appropriate basis!)

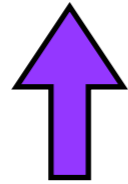
$$\text{Det}(M[\sigma]) = |\text{Det}(D[\sigma])|^2$$

which proves that $\text{Det}(M[\sigma])$ is positive

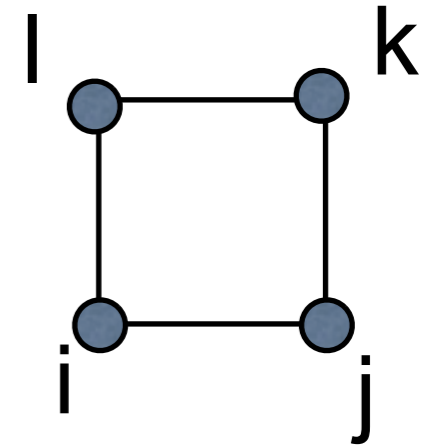
Many interesting problems are not of this type!

Example : A Plaquette model

$$S = \sum_{xy} \bar{\psi}_x M_{xy} \psi_y - g \sum_{\langle ijkl \rangle} (-\bar{\psi}_i \psi_i) (-\bar{\psi}_j \psi_j) (-\bar{\psi}_k \psi_k) (-\bar{\psi}_l \psi_l)$$



has a "solvable" form



$$Z = \int [d\bar{\psi}\psi] e^{-\bar{\psi}M\psi} \prod_{\langle ijkl \rangle} e^{g(-\bar{\psi}_i \psi_i) (-\bar{\psi}_j \psi_j) (-\bar{\psi}_k \psi_k) (-\bar{\psi}_l \psi_l)}$$

$$e^{g(-\bar{\psi}_i \psi_i) (-\bar{\psi}_j \psi_j) (-\bar{\psi}_k \psi_k) (-\bar{\psi}_l \psi_l)} = \sum_{z_{ijkl} \in \mathbb{Z}_4} e^{g^{1/4} z_{ijkl} \sum_{a=i,j,k,l} (-\bar{\psi}_a \psi_a)}$$

$$Z = \sum_{[z]} \int [d\bar{\psi}d\psi] e^{-\bar{\psi}_i (M_{ij} + g^{1/4} \bar{z} \delta_{ij}) \psi_j}$$



leads to sign problems

Lesson

Introducing Auxiliary fields without thought can lead to sign problems!

Are there other ways
to approach the Grassmann Integration
beyond the “traditional approach”?

A new look at Grassmann Integration

Grassmann numbers help generate fermion “worldlines”

$$\bar{\psi}_i \psi_j = \text{---} \circ \xrightarrow{\quad} \circ \text{---}$$

(Diagram: A horizontal purple arrow pointing from a purple dot labeled 'i' to a purple dot labeled 'j'. Below each dot is a vertical purple line segment.)

$$\bar{\psi}_i \psi_i = \text{---} \circ \curvearrowright \circ \text{---}$$

(Diagram: A purple dot labeled 'i' with a purple arrow forming a clockwise loop around it. Below the dot is a vertical purple line segment.)

$$\bar{\psi}_i \psi_j \bar{\psi}_j \psi_i = \text{---} \circ \begin{array}{c} \curvearrowright \\ \curvearrowleft \end{array} \circ \text{---}$$


(Diagram: Two purple dots labeled 'i' and 'j' with two purple arrows forming a closed loop between them. Below each dot is a vertical purple line segment.)

$$e^{\eta_{ij} \bar{\psi}_i \psi_j} = 1 + \eta_{ij} \bar{\psi}_i \psi_j = \text{---} \circ \quad \circ \text{---} + \eta_{ij} \text{---} \circ \xrightarrow{\quad} \circ \text{---}$$

(Diagram: The expansion of the exponential function. The first term is '1' (represented by two vertical purple lines at 'i' and 'j'). The second term is η_{ij} times a horizontal purple arrow from 'i' to 'j' (with vertical purple lines below each dot).)

Grassmann Integration is trivial

$$\int d\psi = 0, \quad \int d\psi \psi = 1$$

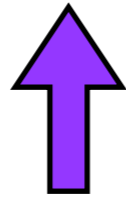
$$\int [d\bar{\psi}_i d\psi_i] \text{ (loop at } i \text{)} = -1$$
A diagram showing a single site labeled 'i' with a purple dot. A purple arrow starts at the dot, goes clockwise in a small circle, and returns to the dot.

$$\int [d\bar{\psi}_j d\psi_j] [d\bar{\psi}_i d\psi_i] \text{ (loop between } i \text{ and } j \text{)} = -1$$
A diagram showing two sites labeled 'i' and 'j' with purple dots. Two purple arrows form a closed loop: one arrow goes from site 'i' to site 'j', and another arrow goes from site 'j' back to site 'i'.

**Every site must have one incoming
and one outgoing line**

Every closed loop gives a -1

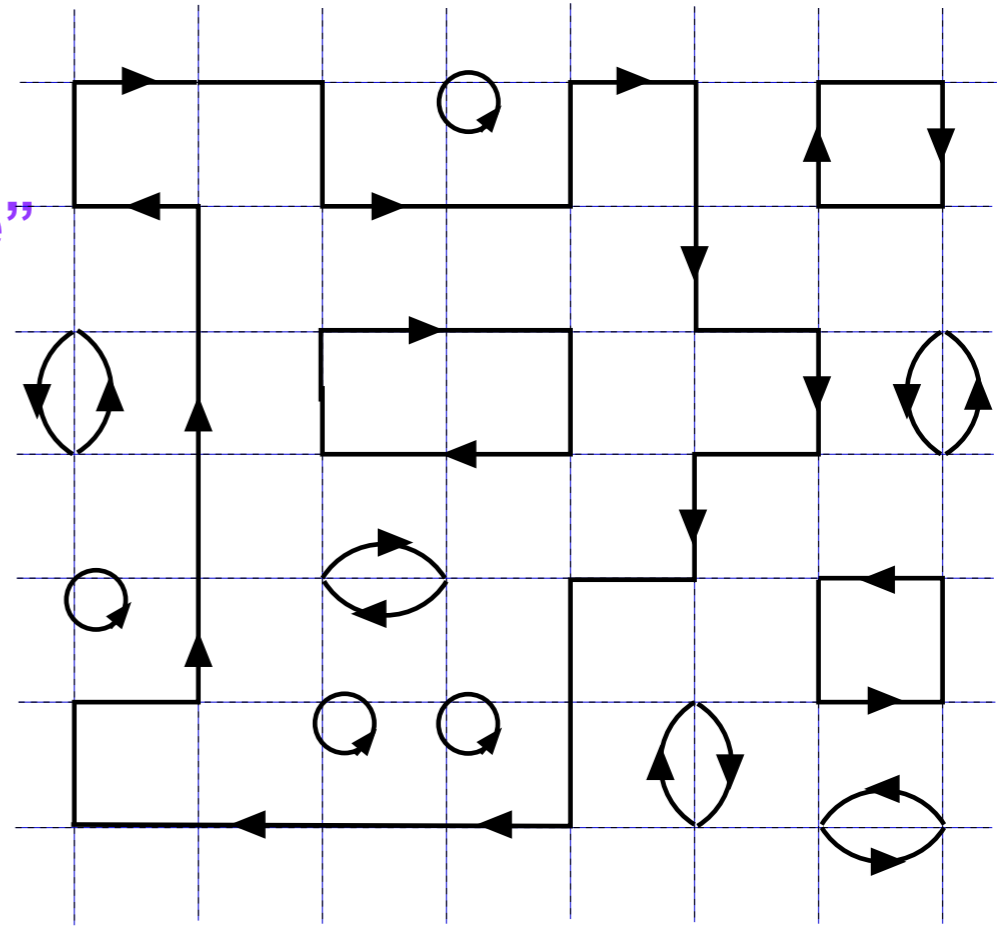
$$\int [d\bar{\psi}d\psi] e^{-\bar{\psi}_i M_{ij} \psi_j} = \sum_C W(C) \text{Sign}(C) = \text{Det}(M)$$



Sum over fermion "worldline"
Configuration

**Weight of
the configuration comes
from local weights of
bonds**

**Sign of a configuration
comes from
local sign factors
and number of loops**



example of C

Fermion Bag Idea

SC, 2010

Group fermion “worldlines”
inside regions called fermion bags
and sum over them

Choose fermion bags carefully
such that the sum (“path integral”) is positive

(Extension of the meron cluster idea)

SC, Wiese, 2000

Consider

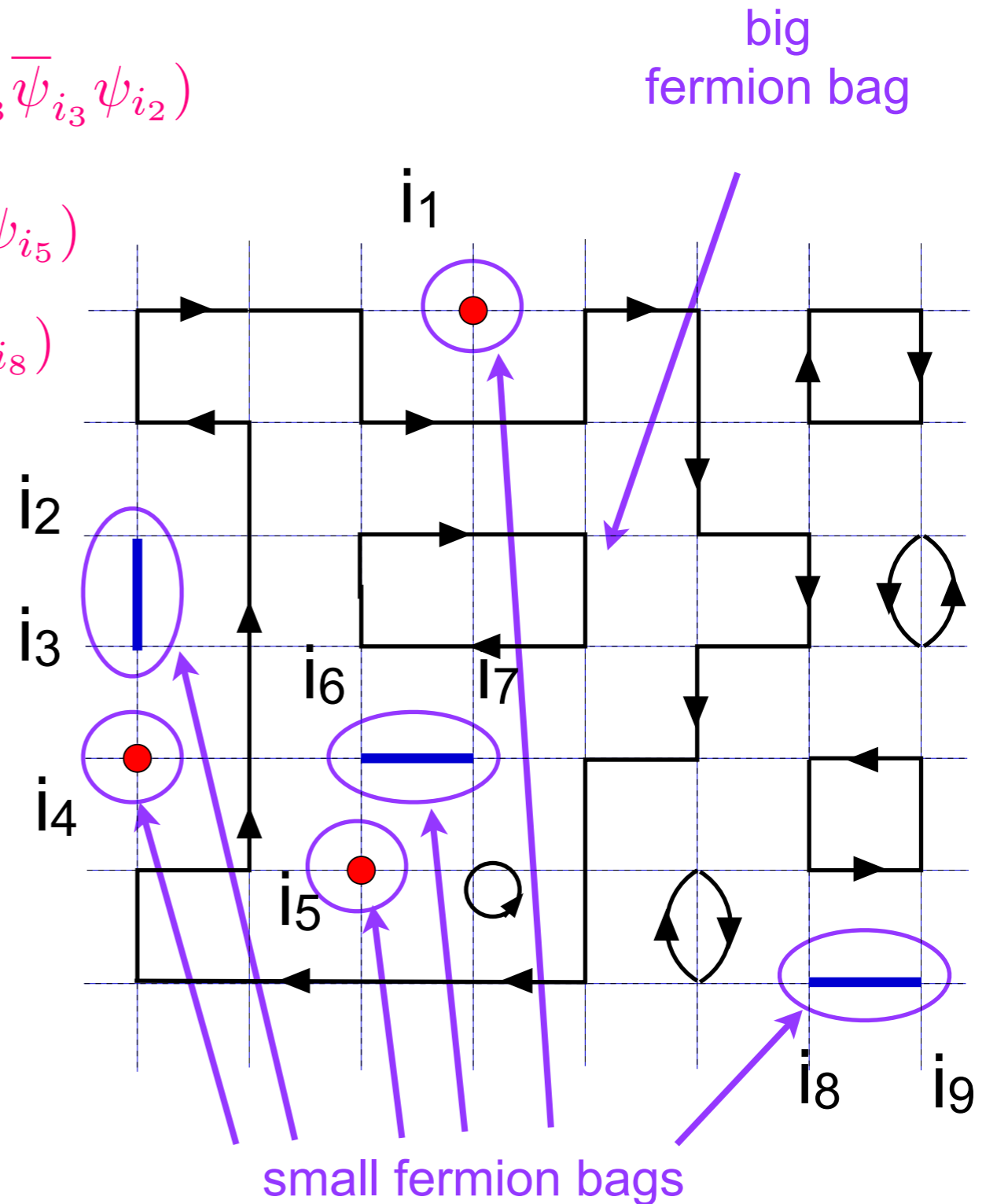
$$\int [d\bar{\psi}d\psi] e^{-\bar{\psi}_i M_{ij} \psi_j} (-\bar{\psi}_{i_1} \psi_{i_1}) (-\bar{\psi}_{i_2} \psi_{i_3} \bar{\psi}_{i_3} \psi_{i_2})$$

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

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

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

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

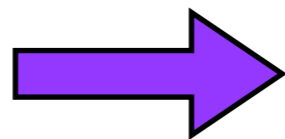


Thus if

$$M = \begin{pmatrix} 0 & D \\ -D^\dagger & 0 \end{pmatrix}$$

then

$$W = \begin{pmatrix} 0 & \tilde{D} \\ -\tilde{D}^\dagger & 0 \end{pmatrix}$$



$$\text{Det}(W) \geq 0$$

This means that theories of the type

$$\begin{aligned} S = & \sum_{ij} \bar{\psi}_i M_{ij} \psi_j - \sum_i U_i (-\bar{\psi}_i \psi_i) \\ & - \sum_{i_1 i_2} U_{i_1 i_2} (-\bar{\psi}_{i_1} \psi_{i_1}) (-\bar{\psi}_{i_2} \psi_{i_2}) + \dots \\ & - \sum_{i_1 \dots i_k} U_{i_1 \dots i_k} (-\bar{\psi}_{i_1} \psi_{i_1}) \dots (-\bar{\psi}_{i_k} \psi_{i_k}) + \dots \end{aligned}$$

have no sign problems as long as
the couplings U are all positive and M is
in the “solvable form”

Can introduce high order fermion couplings easily!

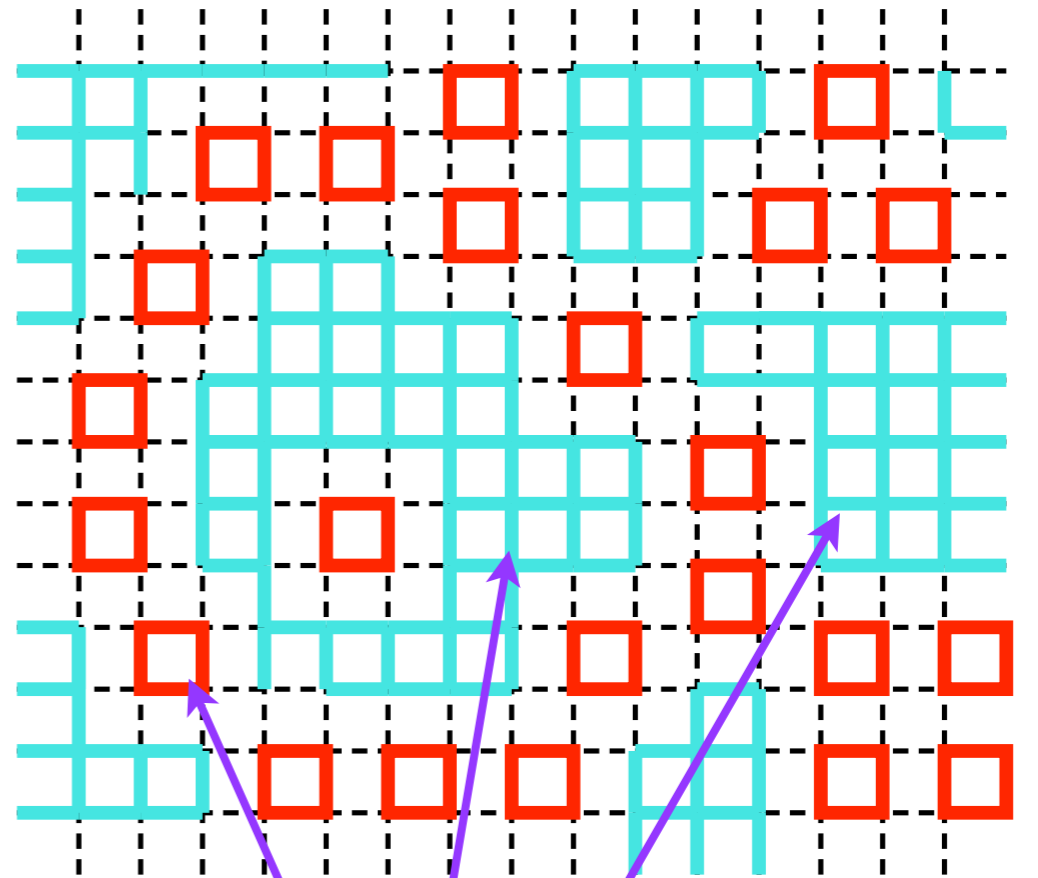
Fermion Bag approach to the plaquette model

$$\begin{aligned}
 Z &= \int [d\bar{\psi}\psi] e^{-\bar{\psi}M\psi} \prod_{\langle ijkl \rangle} e^{g(-\bar{\psi}_i\psi_i)(-\bar{\psi}_j\psi_j)(-\bar{\psi}_k\psi_k)(-\bar{\psi}_l\psi_l)} \\
 &= \int [d\bar{\psi}d\psi] e^{-\bar{\psi}_i M_{ij} \psi_j} \prod_{\langle ijkl \rangle} [1 + g(-\bar{\psi}_i\psi_i)(-\bar{\psi}_j\psi_j)(-\bar{\psi}_k\psi_k)(-\bar{\psi}_l\psi_l)] \\
 &= \int [d\bar{\psi}d\psi] e^{-\bar{\psi}_i M_{ij} \psi_j} \prod_{\langle ijkl \rangle} \sum_{n_{ijkl}=0,1} \left\{ g(-\bar{\psi}_i\psi_i)(-\bar{\psi}_j\psi_j)(-\bar{\psi}_k\psi_k)(-\bar{\psi}_l\psi_l) \right\}^{n_{ijkl}} \\
 &= \sum_{[n_{ijkl}]} g^{N_p} \int [d\bar{\psi}d\psi] e^{-\bar{\psi}_i M_{ij} \psi_j} \left\{ (-\bar{\psi}_i\psi_i)(-\bar{\psi}_j\psi_j)(-\bar{\psi}_k\psi_k)(-\bar{\psi}_l\psi_l) \right\}^{n_{ijkl}} \\
 &= \sum_{[n_{ijkl}]} g^{N_p} \text{Det}(W_{[n]})
 \end{aligned}$$

Fermion Bag Partition Function

$$Z = \sum_{[n_{ijkl}]} g^{N_p} \prod_{i \in \text{blue fbags}} \text{Det}(W_{[n,i]})$$

↑ visualizable configurations ↑ contains fermion physics



fermion bags

Compare with Traditional Partition Function

$$Z = \sum_{[z]} \int [d\bar{\psi}d\psi] e^{-\bar{\psi}_i (M_{ij} + g^{1/4} \bar{z} \delta_{ij}) \psi_j}$$

$$Z = \sum_{[z]} \text{Det}((M + g^{1/4} z))$$

suffers from sign problem
and
difficult to visualize classically



A new class of “solvable” problems

Consider actions of the form

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

solvable complex scalar field space dependent mass term

where the action $S_b[\sigma, \phi]$ is chosen such that the sign problem in the k-pt correlation function

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

is solvable.

Solvable bosonic theories are those
in which we can write

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

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

where the $[n]$ is a monomer field labeling
the location of z_1, z_2, \dots, z_k

and (b, ρ) are “other” bosonic fields
introduced to solve the sign problem.

These class of models are not solvable with the traditional approach

$$S = \bar{\psi}(M[\sigma] + g\Phi)\psi + S_b(\sigma, \phi)$$

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

$$Z = \int [d\sigma d\phi] e^{-S_b[\sigma, \phi]} \text{Det}(M[\sigma] + g\Phi)$$

↑
suffers from sign problem

The Fermion bag approach solves the sign problem!

Fermion Bag approach

Rewrite the partition function as

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

Due to the Grassmann nature

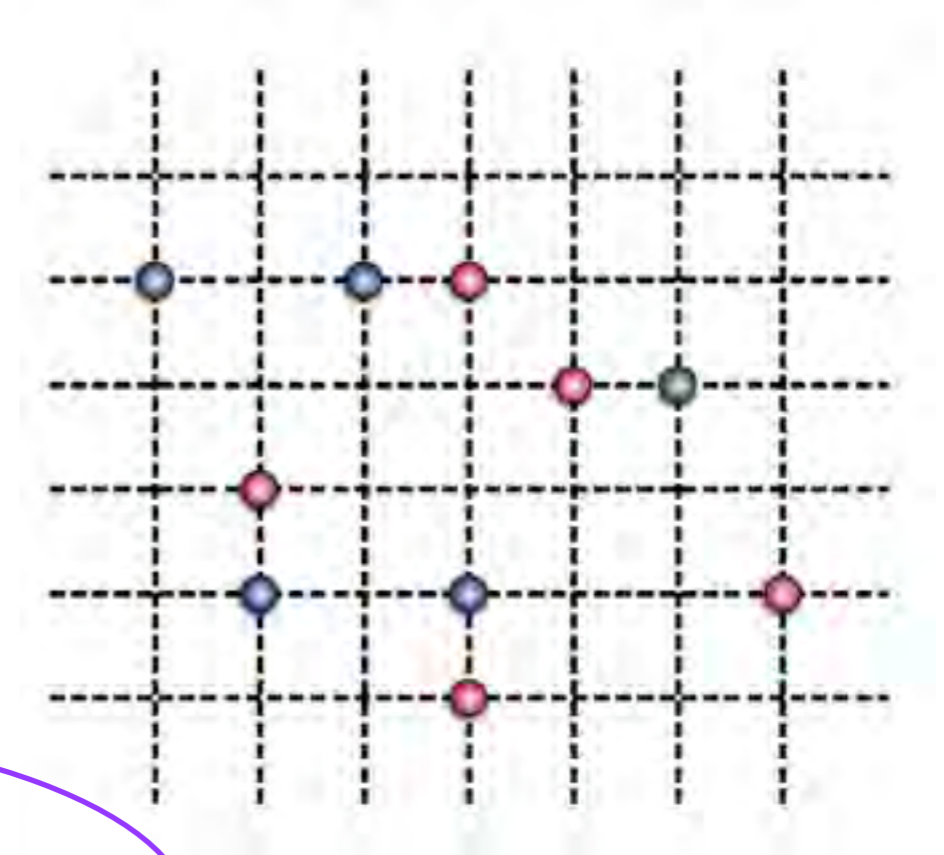
$$e^{-g \phi_x \bar{\psi}_x \psi_x} = 1 + g \phi_x (-\bar{\psi}_x \psi_x) = \sum_{n_x=0,1} \left(g \phi_x (-\bar{\psi}_x \psi_x) \right)^{n_x}$$

We can then rewrite

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

example of configuration [n] with k = 10

For a given configuration [n]
 let $z_1 z_2 \dots z_k$ be the k sites
 where $n_x = 1$
 at all other sites $n_x = 0$



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

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

$$\int [d\bar{\psi} d\psi] e^{-\bar{\psi} M[\sigma] \psi} (-\bar{\psi}_{z_1} \psi_{z_1}) (-\bar{\psi}_{z_2} \psi_{z_2}) \dots (-\bar{\psi}_{z_k} \psi_{z_k})$$

Fermion Correlation Function?

Fermion k-point correlation function

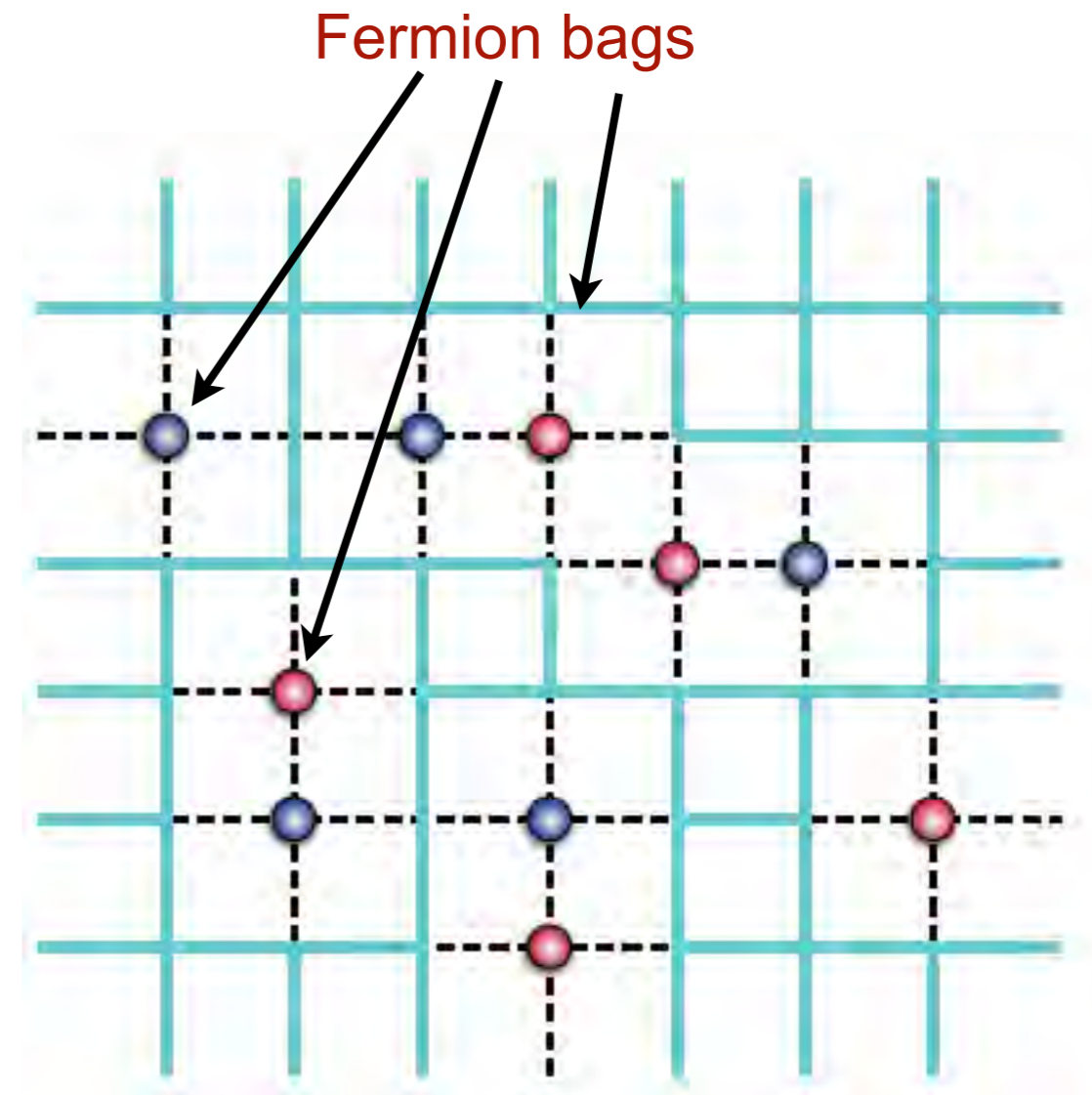
$$\int [d\bar{\psi}d\psi] e^{-\bar{\psi} M[\sigma] \psi} \bar{\psi}_{z_1} \psi_{z_1} \dots \bar{\psi}_{z_k} \psi_{z_k}$$

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

W is a $(V-k) \times (V-k)$ matrix
obtained by dropping sites $z_1 \dots z_k$ in M

$$M[\sigma] = \begin{pmatrix} 0 & D[\sigma] \\ -D^\dagger[\sigma] & 0 \end{pmatrix}$$

$$W[n, \sigma] = \begin{pmatrix} 0 & w[n, \sigma] \\ -w^\dagger[n, \sigma] & 0 \end{pmatrix}$$



fermion bag configuration

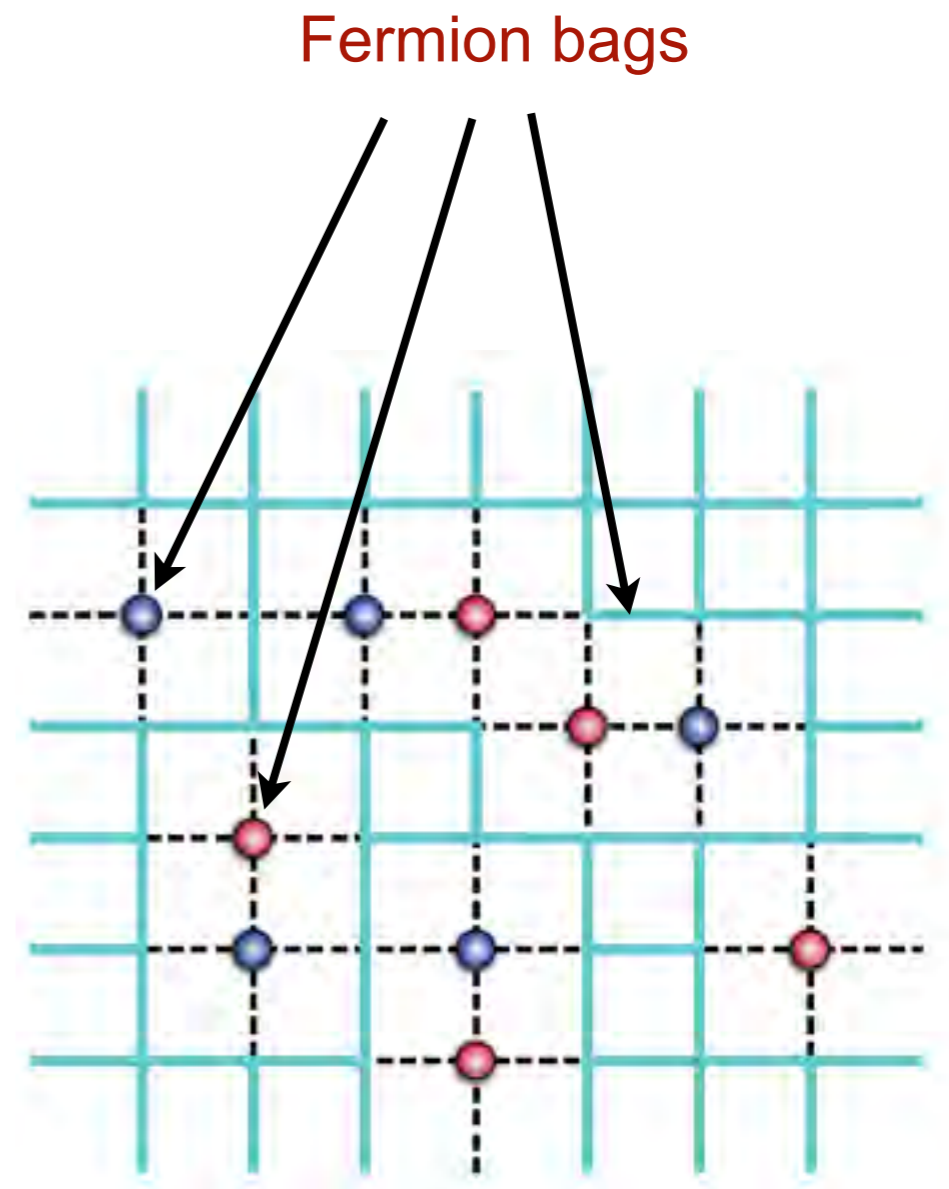
Thus, the partition function
is given by

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



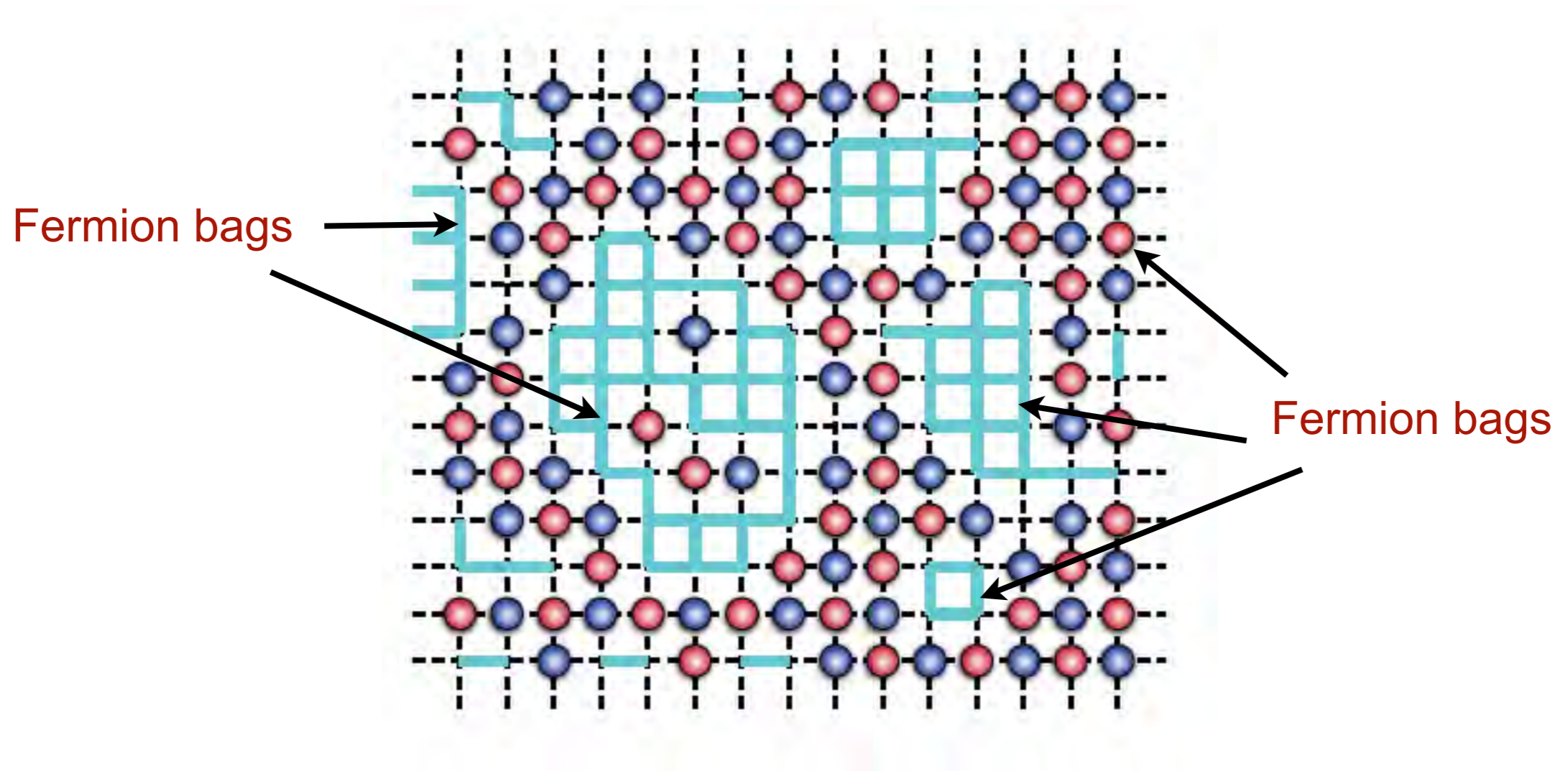
No sign problem!

Mapping into
classical statistical mechanics



fermion bag configuration

At large coupling --> many small fermion bags



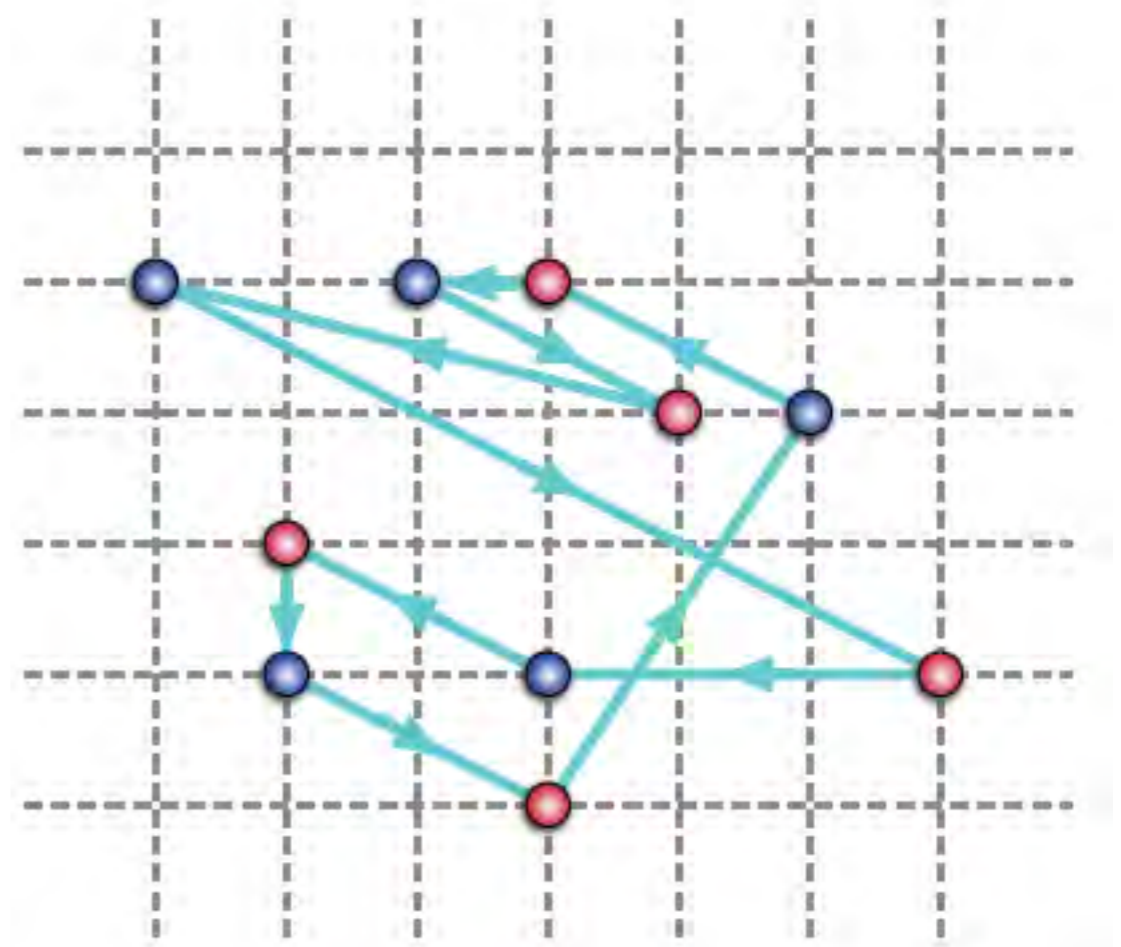
small fermion bags --> computation is efficient!

Duality

k-point correlation function

$$\int [d\bar{\psi}d\psi] e^{-\bar{\psi} M[\sigma] \psi} \bar{\psi}_{z_1} \psi_{z_1} \dots \bar{\psi}_{z_k} \psi_{z_k} = \text{Det}(M[\sigma]) \text{Det}(G_{[n]}(\sigma))$$

where $G_{[n]}$ is a $(k \times k)$ matrix of propagators



Dual Fermion Bag

Rubtsov, Savkin, Lichtenstein, Prokofev, Svistunov, Troyer, ...

Duality Relation

$$\text{Det } W^0 = \text{Det } D^0 \text{ Det } G_{[n]}$$



strong coupling
fermion bag



weak coupling
fermion Bag

diagrammatic
determinantal Monte Carlo

Lesson

A sign problem can be entangled in both fermionic and bosonic variables.

A full solution may require one to solve the sign problems in both the variables!

“Solvable” problems with spin-half

$$S = \sum_{xy} \bar{\psi}_x M_{xy} \psi_x + g \sum_x (\phi_x \psi_{\uparrow,x} \psi_{\downarrow,x} + \phi_x^* \bar{\psi}_{\downarrow,x} \bar{\psi}_{\uparrow,x}) + S_b$$

If $\sigma_2 M \sigma_2 = M^*$ then $\text{Det}(M) \geq 0$

It is then possible to argue that $\sigma_2 W \sigma_2 = W^*$

so $\text{Det}(W) \geq 0$

Sign problem is solved!

Many interesting lattice field theory models solvable

SU(2) Yukawa models with Wilson Fermions

Gauged NJL models

Models inspired by Graphene

New models with pairing interactions

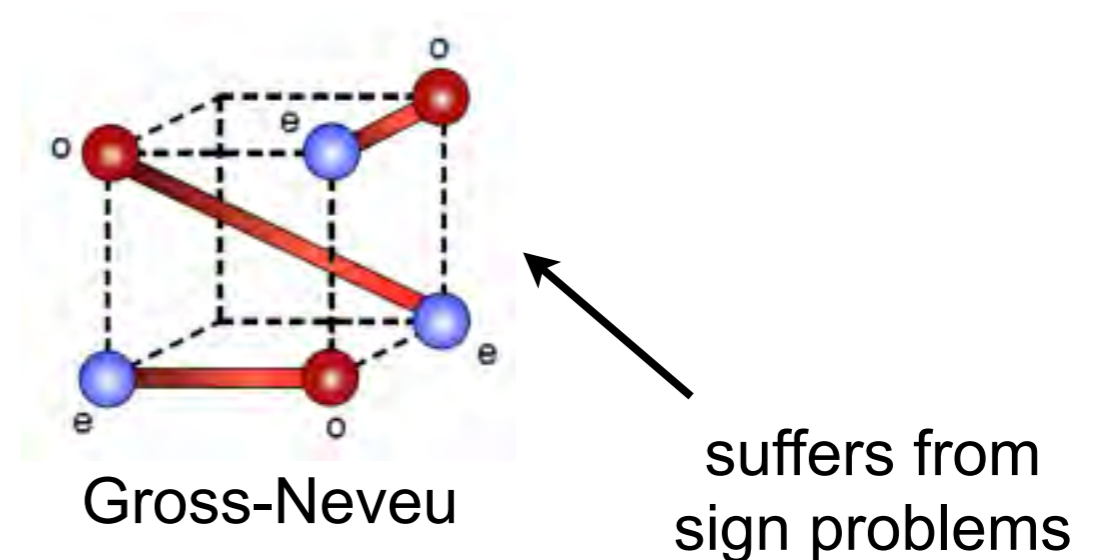
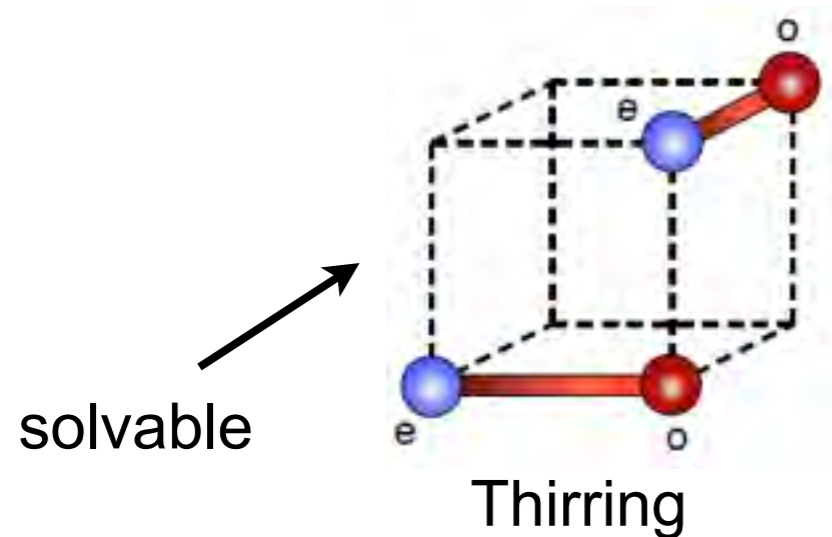
Some models with repulsive interactions also solvable!

Results: “Graphene” Hubbard Models

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

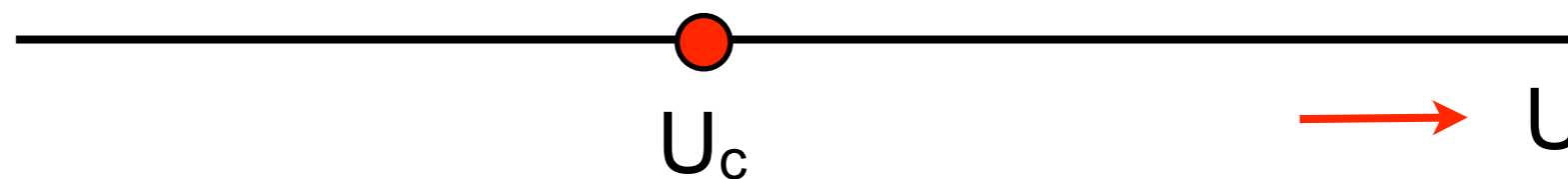
SU(2) x U(1) symmetric models

$$S(\theta, \bar{\psi}, \psi) = \sum_{xy} \bar{\psi}_x M_{xy} \psi_y - \sum_{\langle xy \rangle} U_{\langle xy \rangle} \bar{\psi}_x \psi_x \bar{\psi}_y \psi_y$$



massless fermions/
U(1) symmetric

massive fermions/
U(1) broken



Observables

chiral susceptibility

$$\chi = \left\langle \frac{1}{2L^3} \sum_{\mathbf{x}, \mathbf{y}} \bar{\psi}_{\mathbf{x}} \psi_{\mathbf{x}} \bar{\psi}_{\mathbf{y}} \psi_{\mathbf{y}} \right\rangle$$

chiral winding susceptibility

$$\mathbf{q}_{\chi}^2 = \left\langle \frac{1}{3} \sum_{\alpha} (\mathbf{q}_{\chi}^2)_{\alpha} \right\rangle$$

fermion correlation ratio

$$\mathbf{C}_{\mathbf{F}}(\mathbf{t}) = \left\langle \frac{1}{3} \sum_{\alpha} \bar{\psi}_{\mathbf{0}, \mathbf{0}, \mathbf{0}} \psi_{\mathbf{0}, \mathbf{0}, \mathbf{t}\hat{\alpha}} \right\rangle$$

$$\mathbf{R}_{\mathbf{F}} = \mathbf{C}_{\mathbf{F}}(\mathbf{L}/2 - \mathbf{1}) / \mathbf{C}(\mathbf{1})$$

Critical Finite Size Scaling

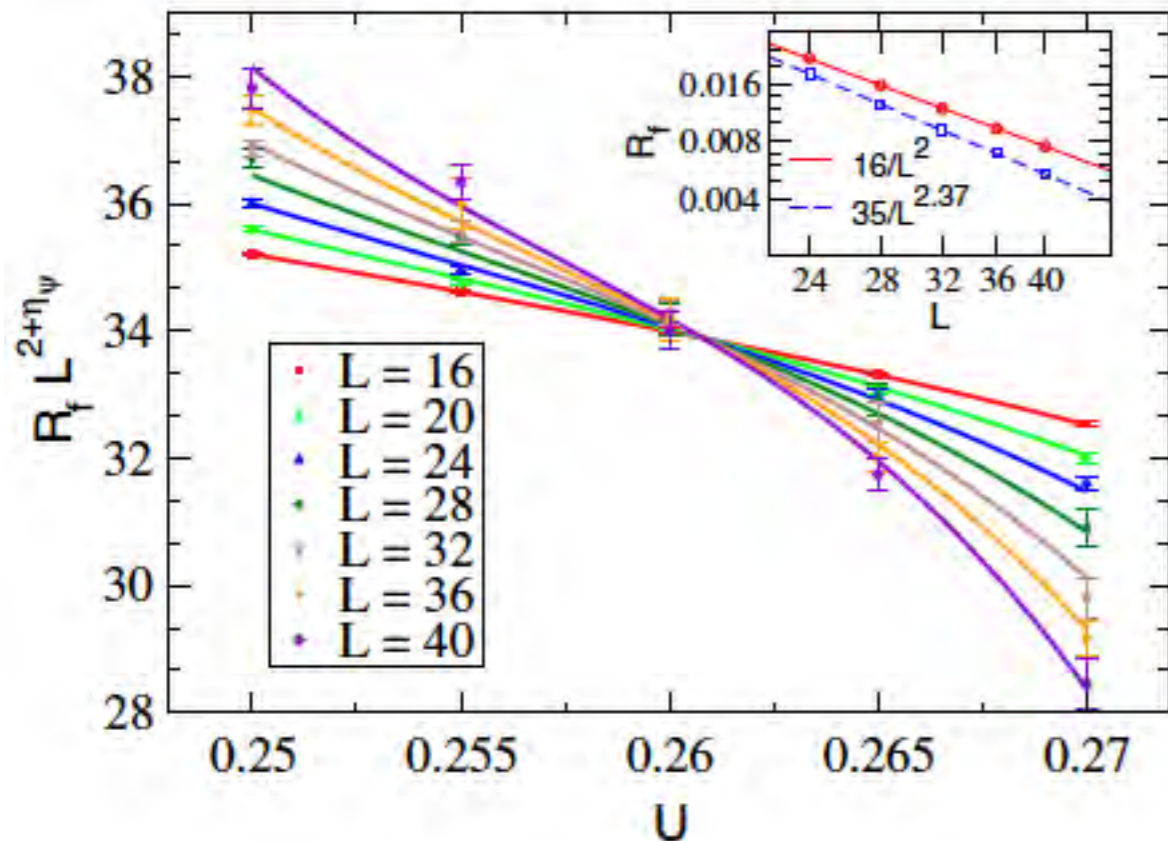
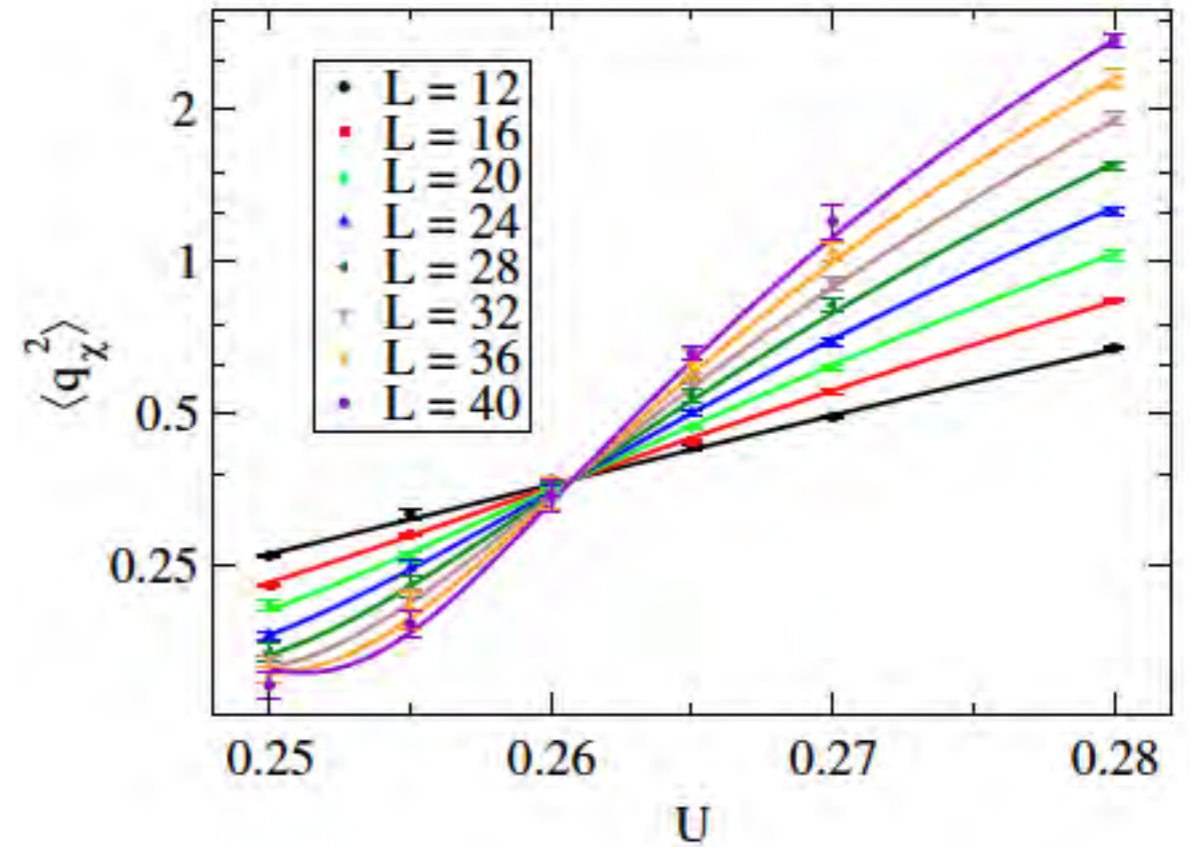
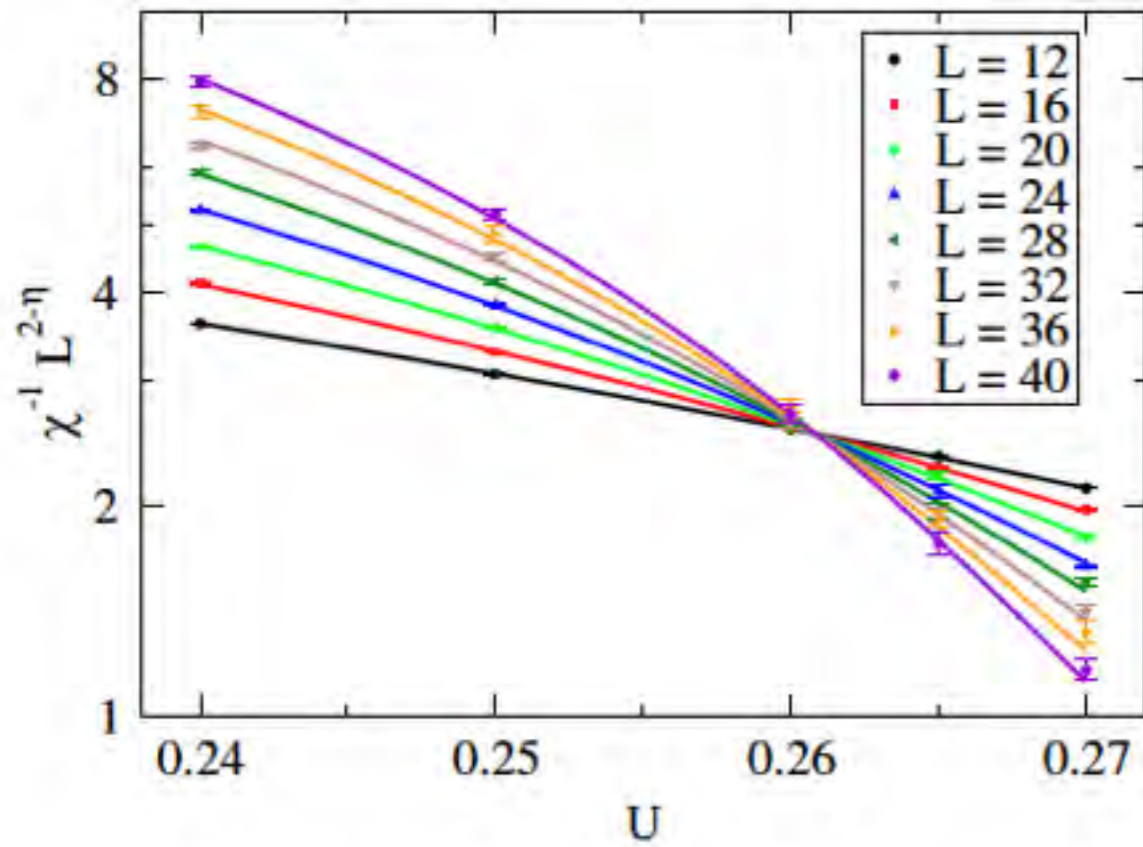
$$\chi^{-1} L^{2-\eta} = f_0 + f_1 (U - U_c) L^{1/\nu} + f_2 (U - U_c)^2 L^{2/\nu} + \dots$$

$$\langle q_\chi^2 \rangle = \kappa_0 + \kappa_1 (U - U_c) L^{1/\nu} + \kappa_2 (U - U_c)^2 L^{2/\nu} + \dots$$

$$R_f L^{2+\eta\psi} = p_0 + p_1 (U - U_c) L^{1/\nu} + p_2 (U - U_c)^2 L^{2/\nu} + \dots$$

If we plot w.r.t U
all quantities must be independent of L at $U = U_c$

Thirring model results



Combined fit results

$$U_c = 0.2608(2)$$

$$v = 0.85(1)$$

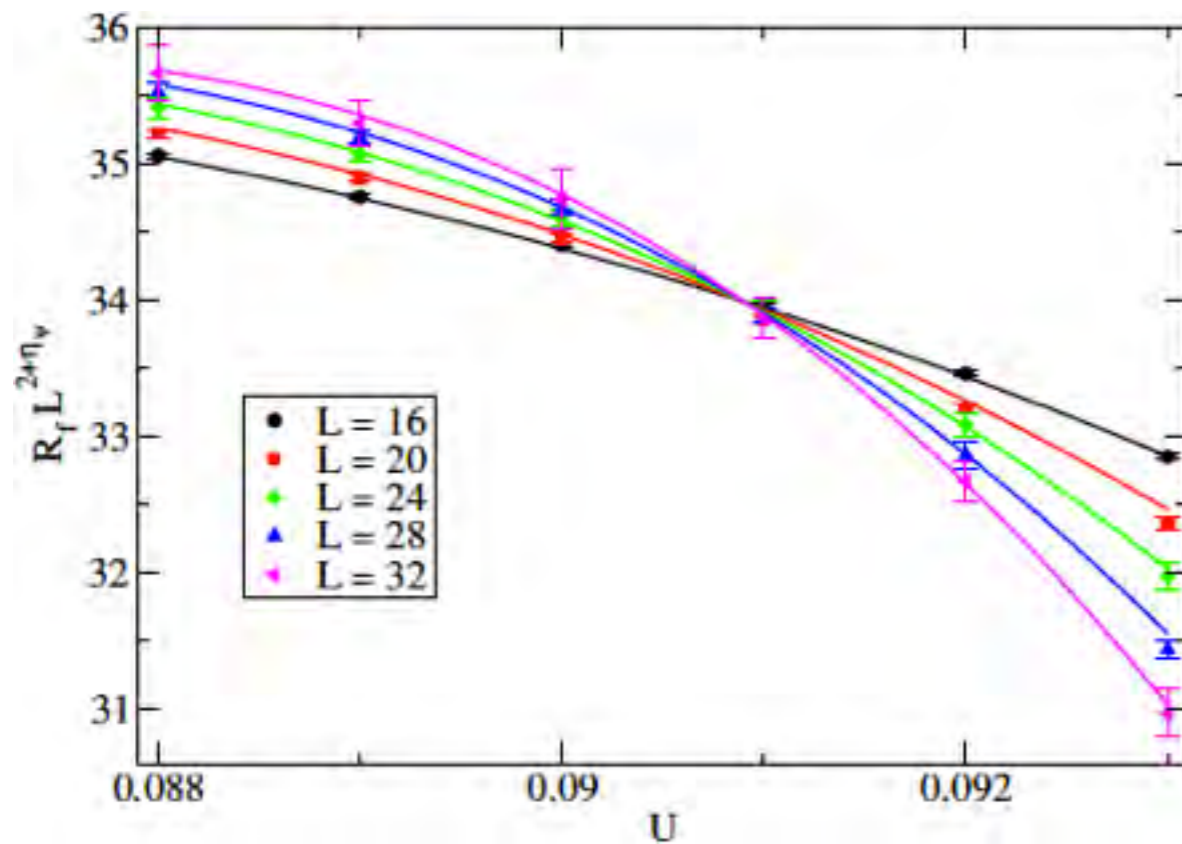
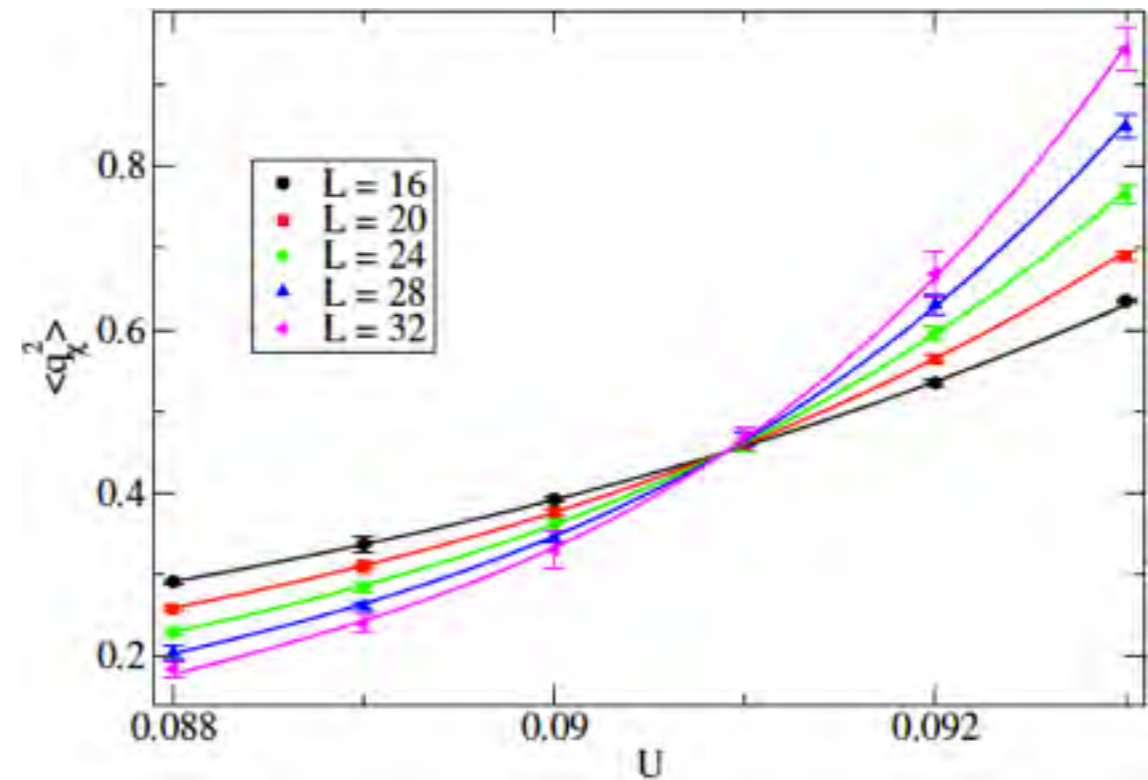
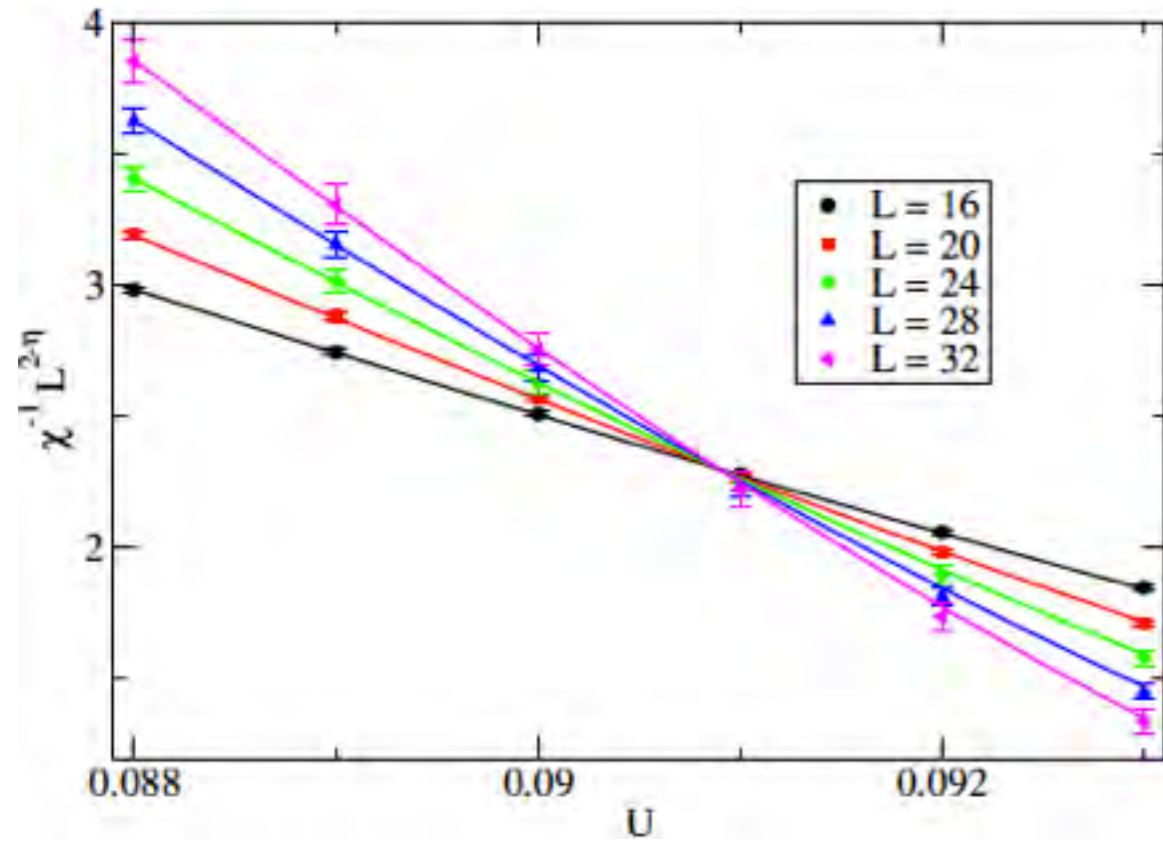
$$\eta = 0.65(1)$$

$$\eta_\psi = 0.37(1)$$

Comparison with previous work

Work	Range of L	Range of m	U_c	v	η	η_Ψ
Mean Field Theory Lee & Shrock PRL (1987)	N/A	0	0.25	1.0	1.0	0.0
Hybrid Monte Carlo Debbio & Hands, PLB (1997)	8-12	0.4-0.02	0.250(10)	0.80(15)	0.7(15)	??
Hybrid Monte Carlo Barbour et. al., PRD (1998)	16-24	0.06-0.01	0.250(06)	0.80(20)	0.4(2)	??
Fermion Bag S.C & A. Li (our work)	12-40	0	0.2608(2)	0.85(1)	0.65(1)	0.37(1)

Gross-Neveu model results



Combined fit results

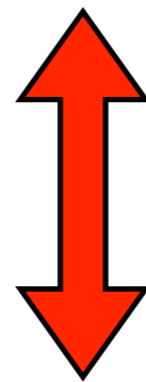
$$U_c = 0.1560(4)$$

$$\nu = 0.82(2)$$

$$\eta = 0.62(2)$$

$$\eta_\psi = 0.37(1)$$

Lattice Thirring Model
(no sign problem in the traditional approach)



same universality class

Lattice GN Model
(complex determinant in traditional approach)

surprising?

ALL previous (traditional) MC results for GN models
are well described by Large N_f
(Christoffi & Strouthos, JHEP(2007))

$$\text{Large } N_f : v = 1, \eta = 1, \eta_\psi = 0$$

Usually involve extra “doubling” to solve sign problems

Belief : Sign problems is NOT a problem in GN models

Our results show clear
deviations with the large N_f results!

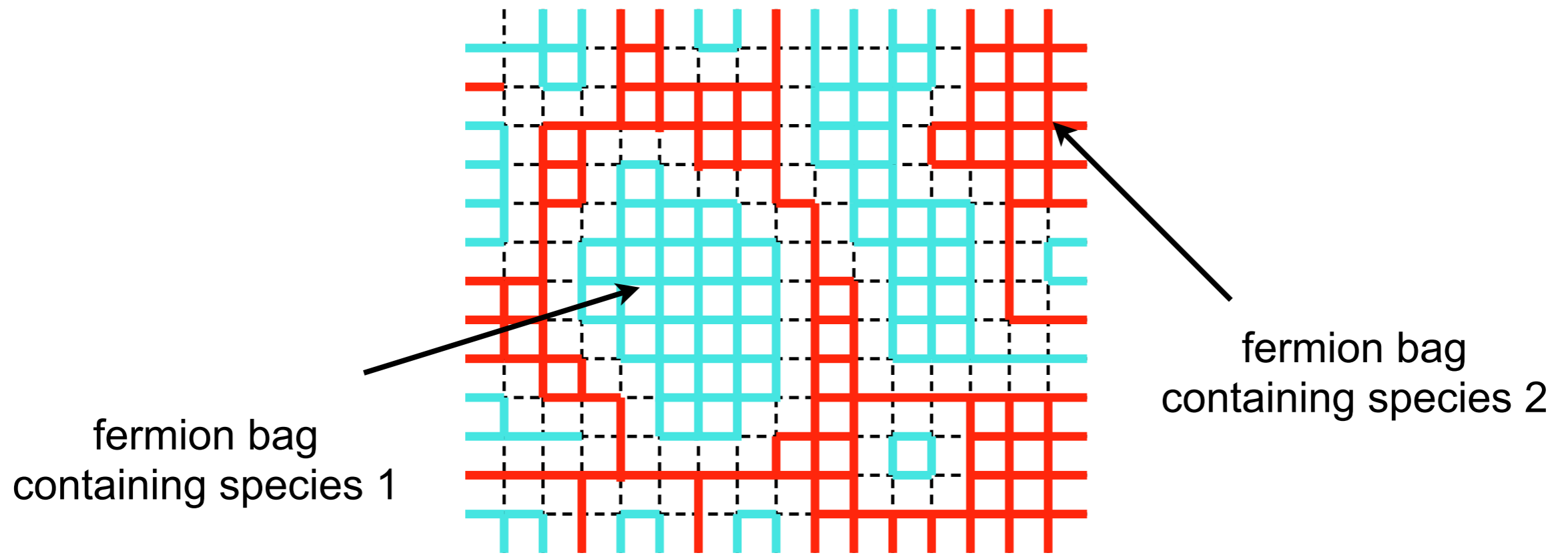
$$v \approx 0.85, \eta \approx 0.65, \eta_\psi \approx 0.37$$

**Our critical exponents in a related model
with $SU(2) \times Z_2$ symmetry
disagrees with earlier work that ignored sign problem!**

Karkkainen, Lacaze, Lacock and Petersson, NPB (1994)

Conclusion : Sign Problem is important!

Two spin-half species model with infinite repulsion



Fermion Bag Configuration

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

Conclusions

Fermion bag approach
is an alternative method to solve
fermion sign problems

Many new sign problems can be solved with it!

Solutions require thought and
understanding of the underlying physics

Solution to sign problems
is an interesting field of research
at the cross roads of
mathematical and computational physics