Fermion-bag approach to strongly correlated fermions

Shailesh Chandrasekharan
(Duke University)

collaborator: Anyi Li (INT, Seattle)
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- Motivation

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- A Lattice Yukawa Model

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- Four-Fermion models

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- Results with massless fermions
- Conclusions

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Strongly correlated fermion systems
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Particle Physics:

Theory of Strong Interactions : QCD

Beyond the standard model physics

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Condensed Matter Physics:

- High Tc Cuprate Materials
- Heavy Fermion Systems
- Graphene

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Beyond the standard model physics

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First Principles Calculations require a
Monte Carlo based method

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The “fermion-bag” approach

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The "fermion-bag" approach

While the new ideas are general,
the new method is currently
only applicable to Yukawa models
(and Four-Fermion models)

Traditional Monte Carlo methods

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Partition function

$$Z = \int [d\phi]\ \mathrm{e}^{-S_b([\phi])} \int [d\overline{\psi}\ d\psi]\ \mathrm{e}^{-\int d^dx\ d^dy\ \overline{\psi}(x) M(x,y;[\phi]) \psi(y)}$$

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Monte Carlo method used to sample [ϕ]

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Singularities :

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$M([\phi])$ is a $V \times V$ matrix
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Singularities :

If $M([\phi])$ contains small or zero eigenvalues,
algorithms like HMC develop singularities

Alternate methods
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Especially methods
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motivation behind current work!

A lattice “Yukawa” model

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Action

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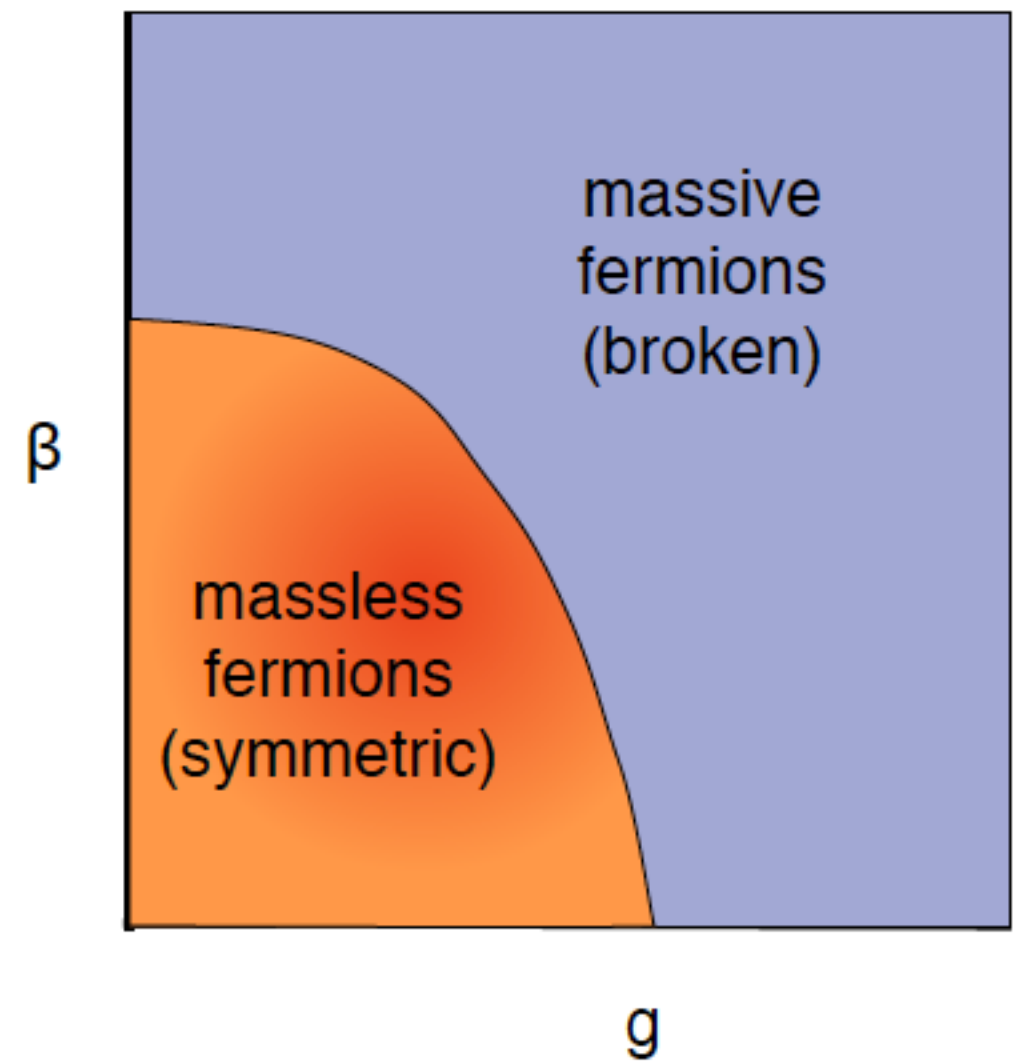
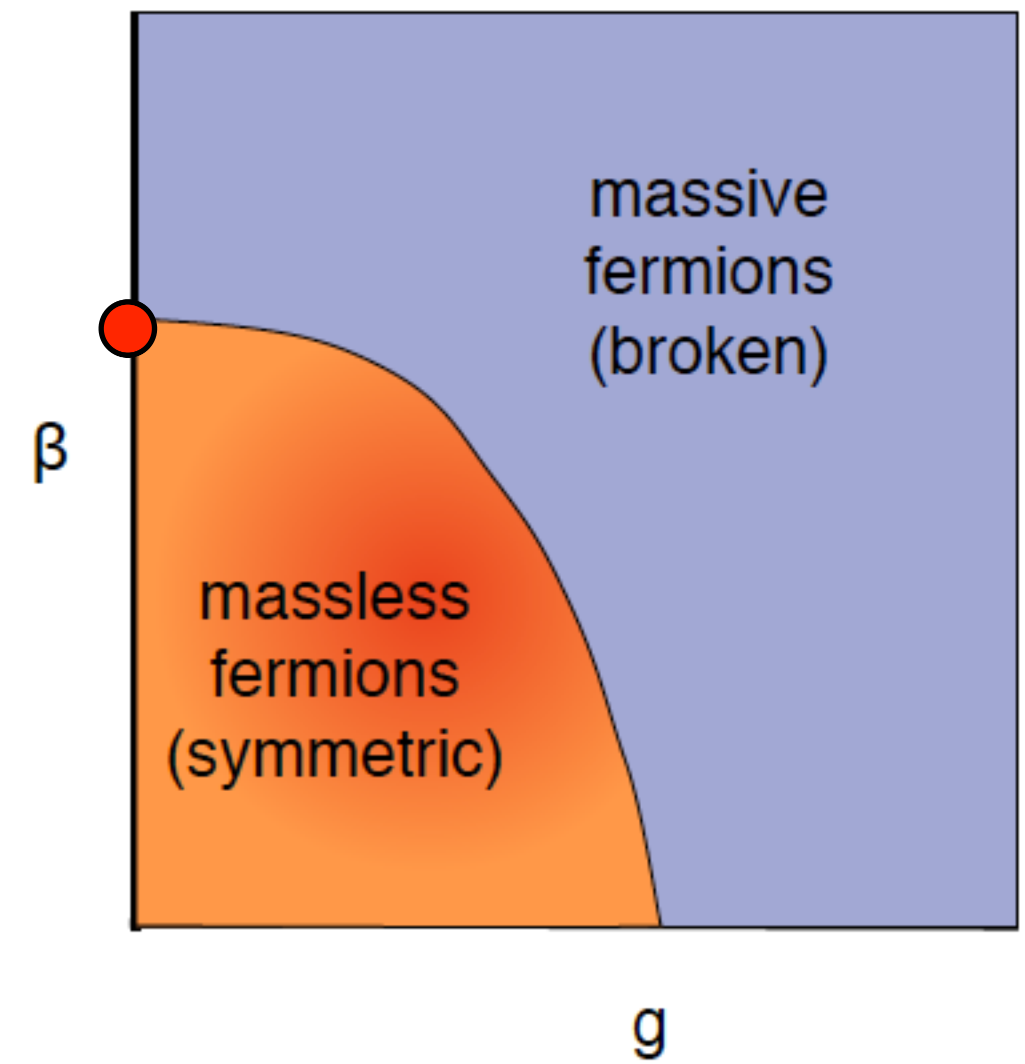
$$\begin{pmatrix} \overline{\psi}_x & \psi_x \end{pmatrix} \to \begin{pmatrix} \overline{\psi}_x & \psi_x \end{pmatrix} \mathbf{S}^{\dagger} \mathrm{e}^{-\mathbf{i}\phi}$$

Phase Diagram

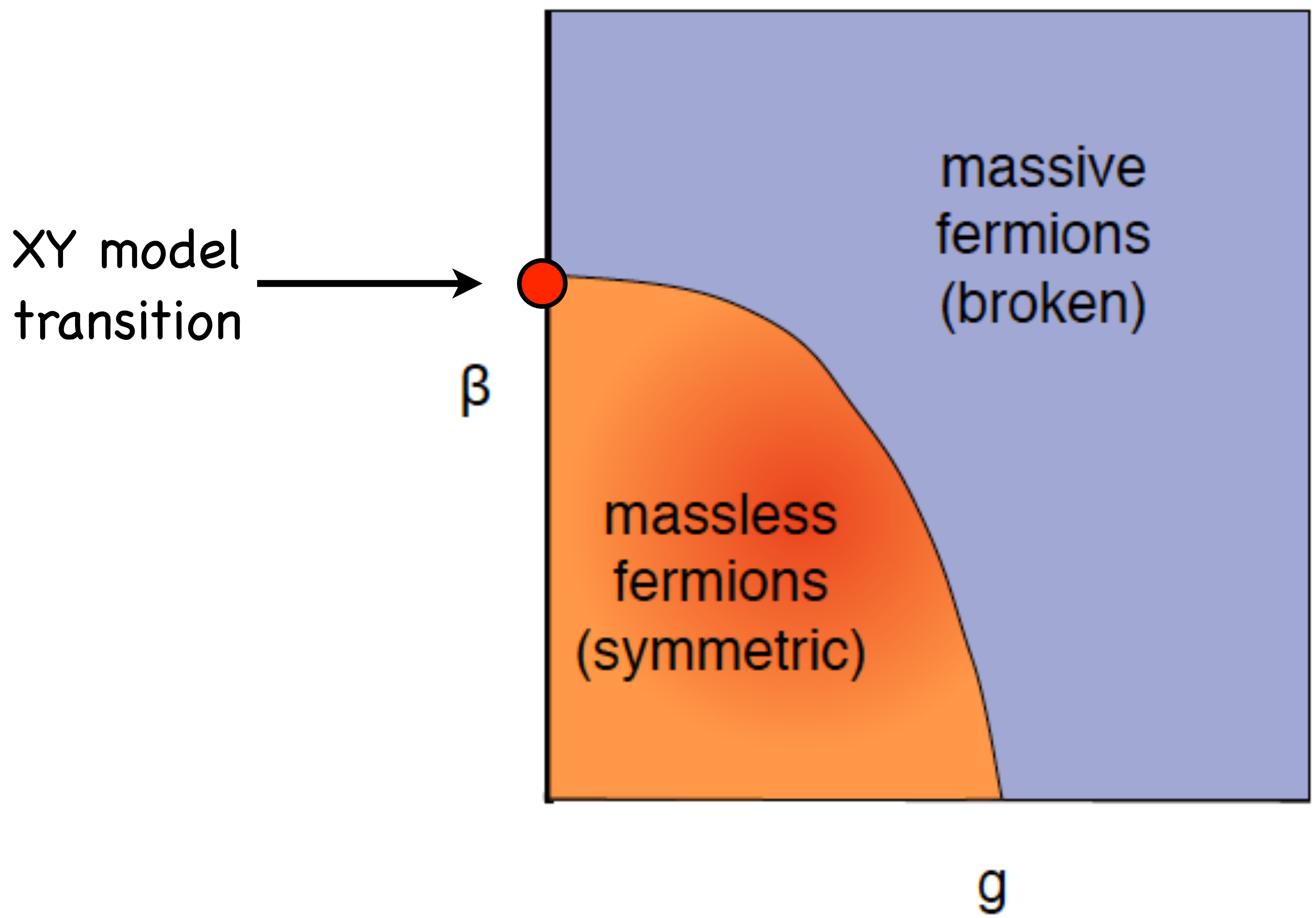
Phase Diagram



Phase Diagram



Phase Diagram



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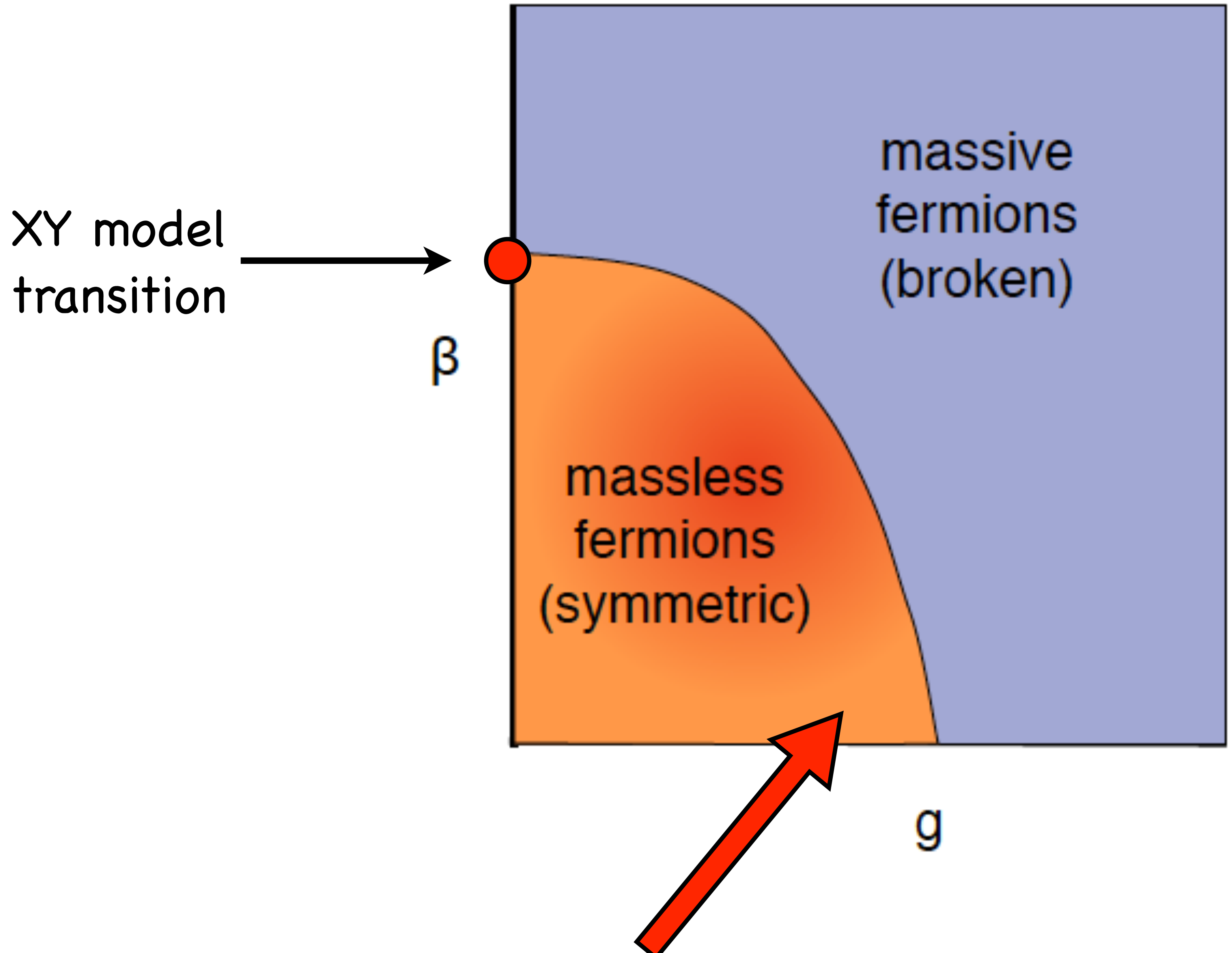
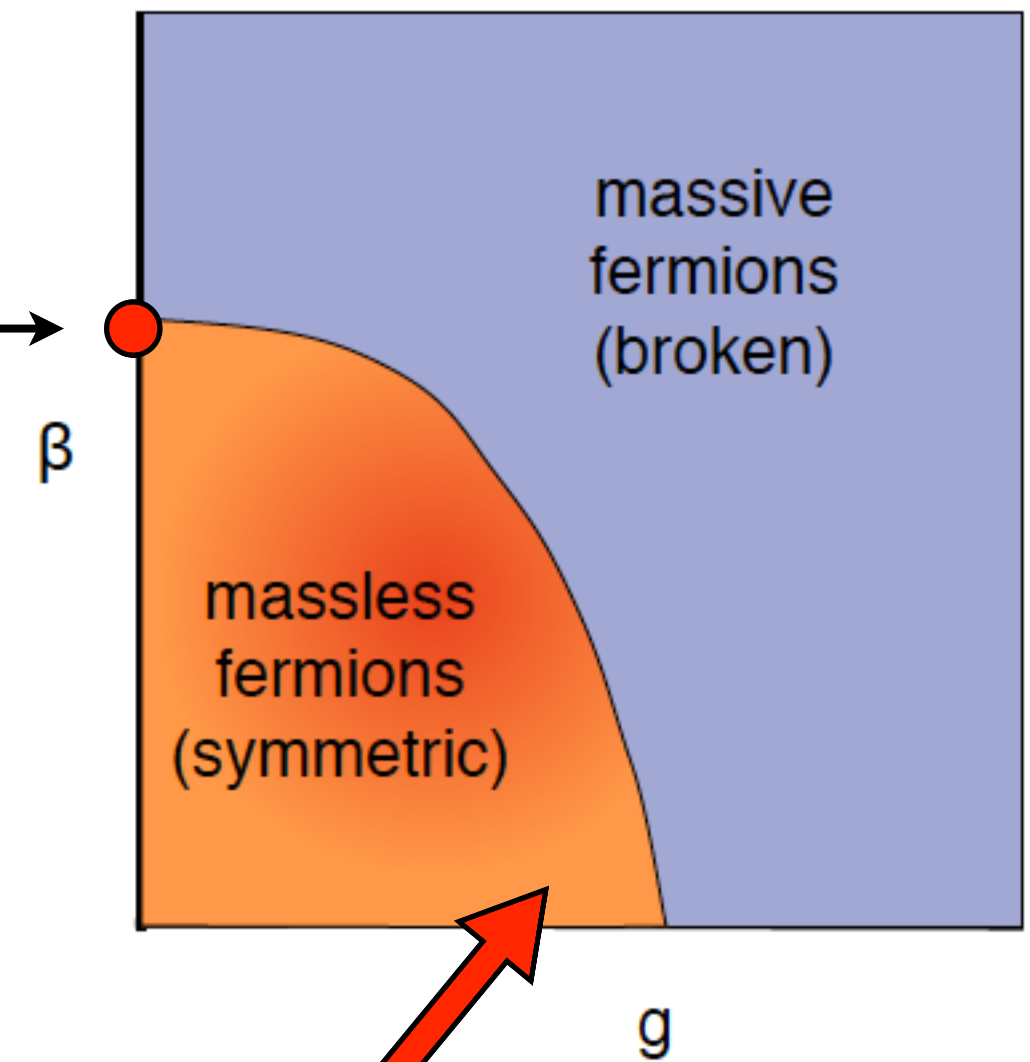


For small β
one gets Four-Fermion models

Phase Diagram

XY model transition



(2+1)d clearly interesting!

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Phase Diagram

XY model
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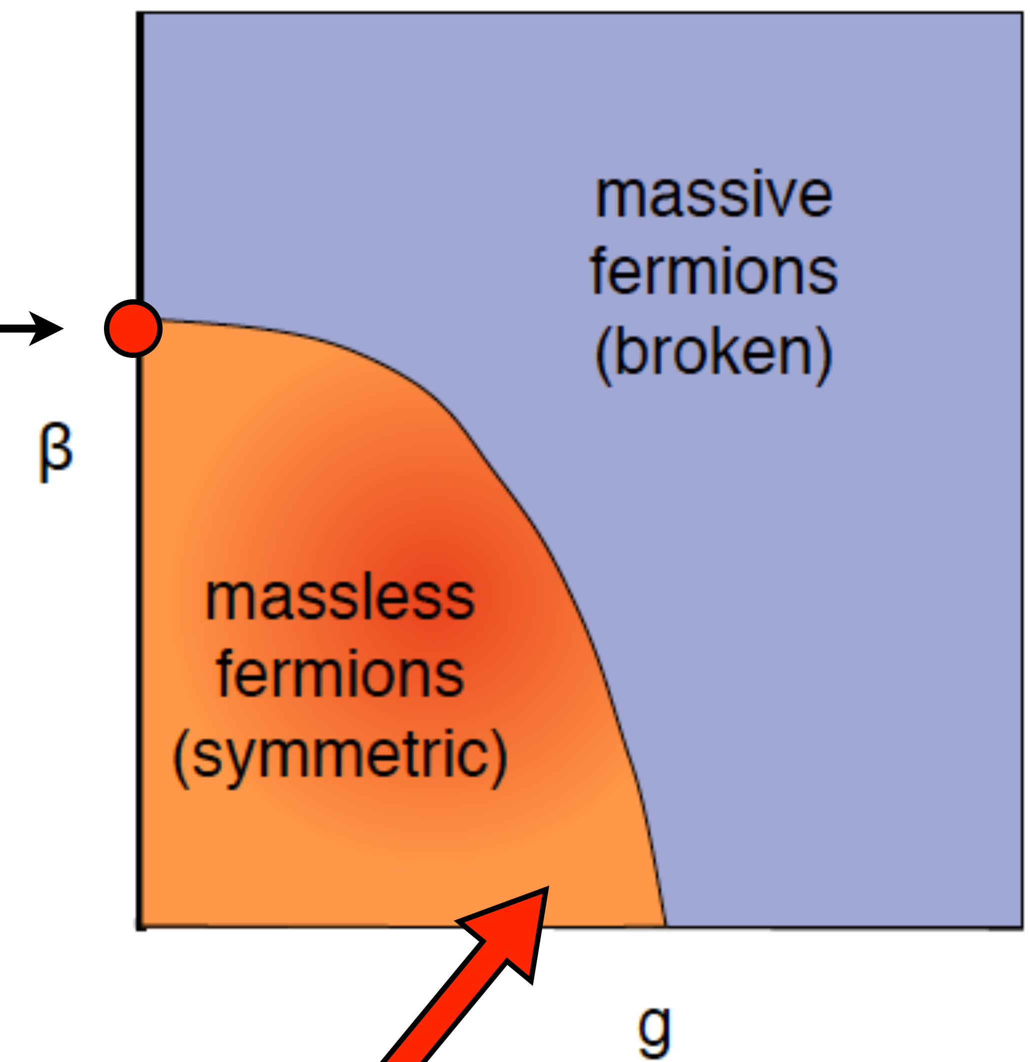

(2+1)d clearly interesting!

(3+1)d may also
be interesting?

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Det(M(Φ)) is complex! --> Severe sign problem

Fermion Bag approach

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S.C PRD(R)(2012)

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Rewrite the partition function as

$$\mathbf{Z} = \int [\mathbf{d}\theta]\left(\prod_{\langle\mathbf{xy}\rangle} \mathrm{e}^{\beta\cos(\theta_{\mathbf{x}}-\theta_{\mathbf{y}})}\right) \int [\mathbf{d}\overline{\psi}\mathbf{d}\psi]\ \mathrm{e}^{-\overline{\psi}\ \mathbf{D^0}\ \psi} \prod_{\mathbf{x}} \left(\mathrm{e}^{\mathbf{g}\ \mathrm{e}^{\mathbf{i}\varepsilon_{\mathbf{x}}\theta_{\mathbf{x}}}\ \overline{\psi}_{\mathbf{x}}\psi_{\mathbf{x}}}\right)$$

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Due to the Grassmann nature

$$\mathrm{e}^{\mathbf{g}\ \mathrm{e}^{\mathbf{i}\varepsilon_{\mathbf{x}}\theta_{\mathbf{x}}}\ \overline{\psi}_{\mathbf{x}}\psi_{\mathbf{x}}} = \mathbf{1} + \mathbf{g}\ \mathrm{e}^{\mathbf{i}\varepsilon_{\mathbf{x}}\theta_{\mathbf{x}}}\overline{\psi}_{\mathbf{x}}\psi_{\mathbf{x}} = \sum_{\mathbf{n_x}=\mathbf{0},\mathbf{1}} \left(\mathbf{g}\ \mathrm{e}^{\mathbf{i}\varepsilon_{\mathbf{x}}\theta_{\mathbf{x}}}\overline{\psi}_{\mathbf{x}}\psi_{\mathbf{x}} \right)^{\mathbf{n_x}}$$

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We can then rewrite

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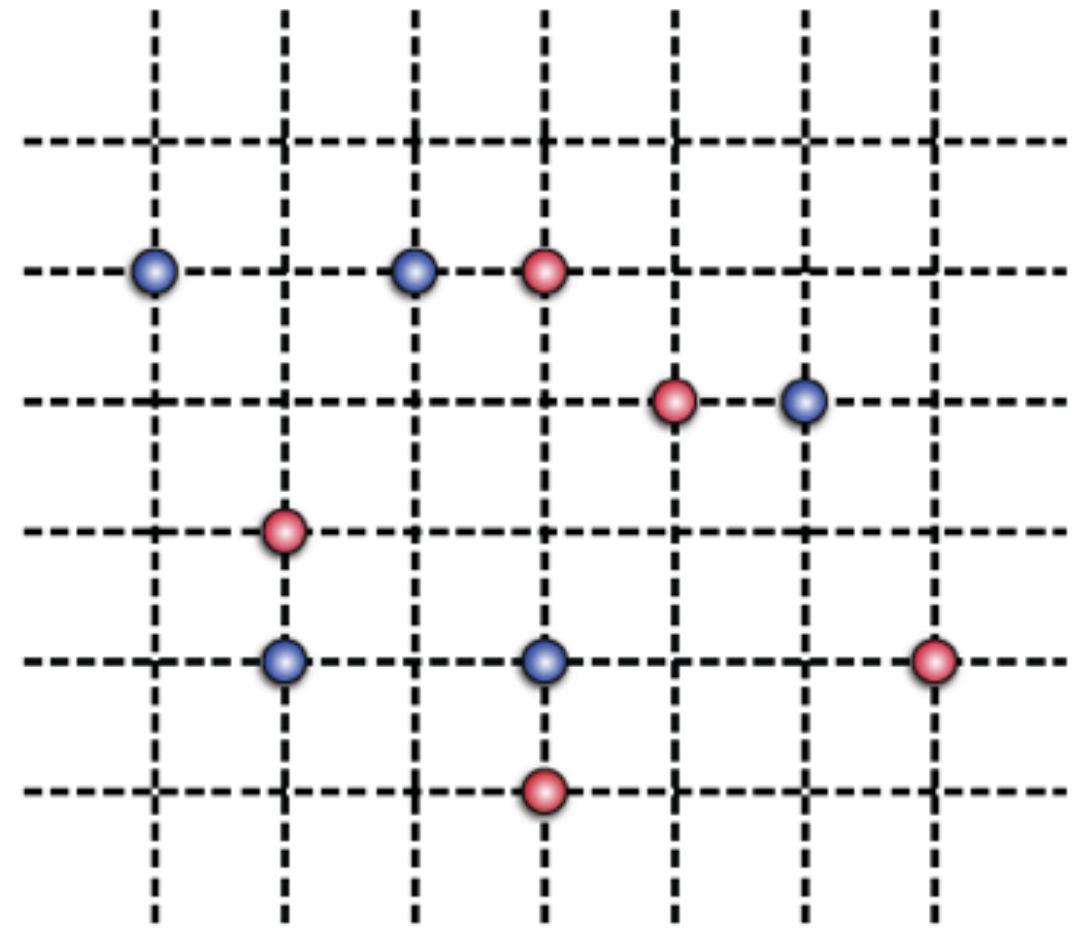
For a given configuration [n]
let z_1 z_2 ... z_k be the k sites
where $n_x = 1$
at all other sites $n_x = 0$

example of configuration $[n_x]$ with $k = 10$



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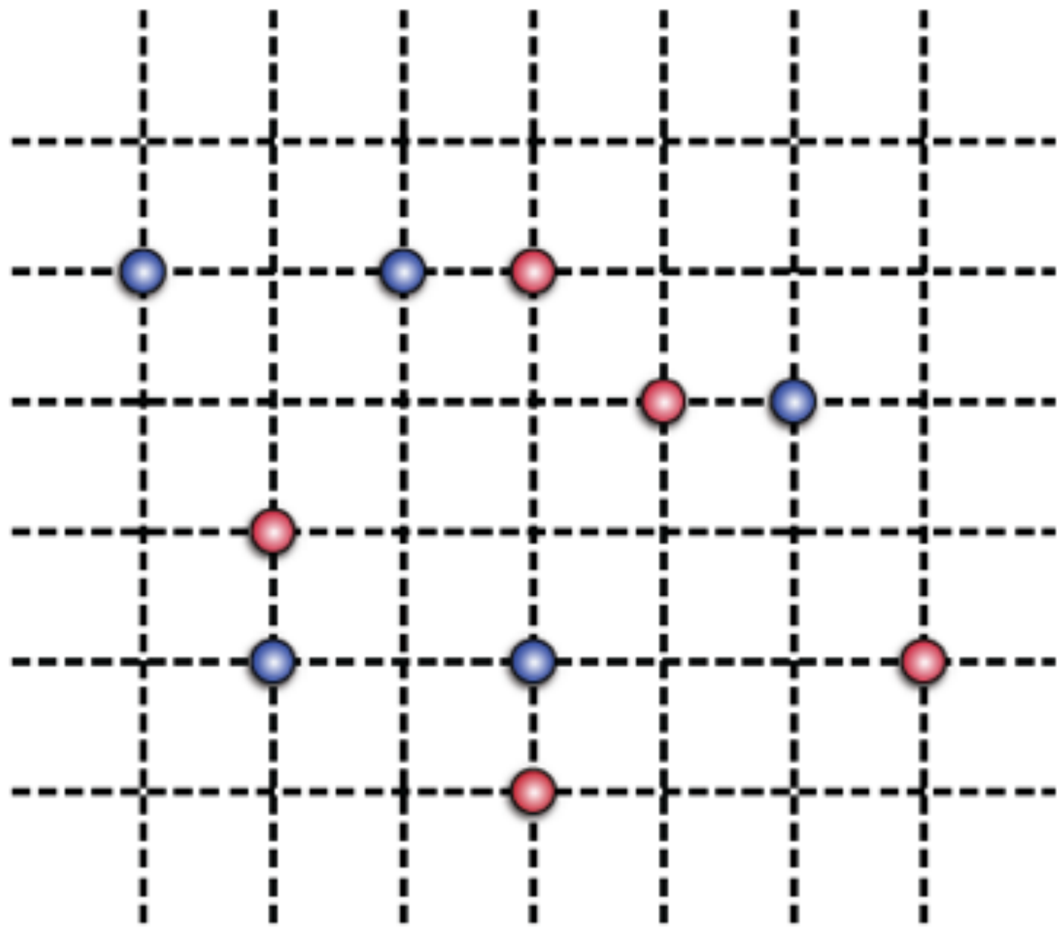

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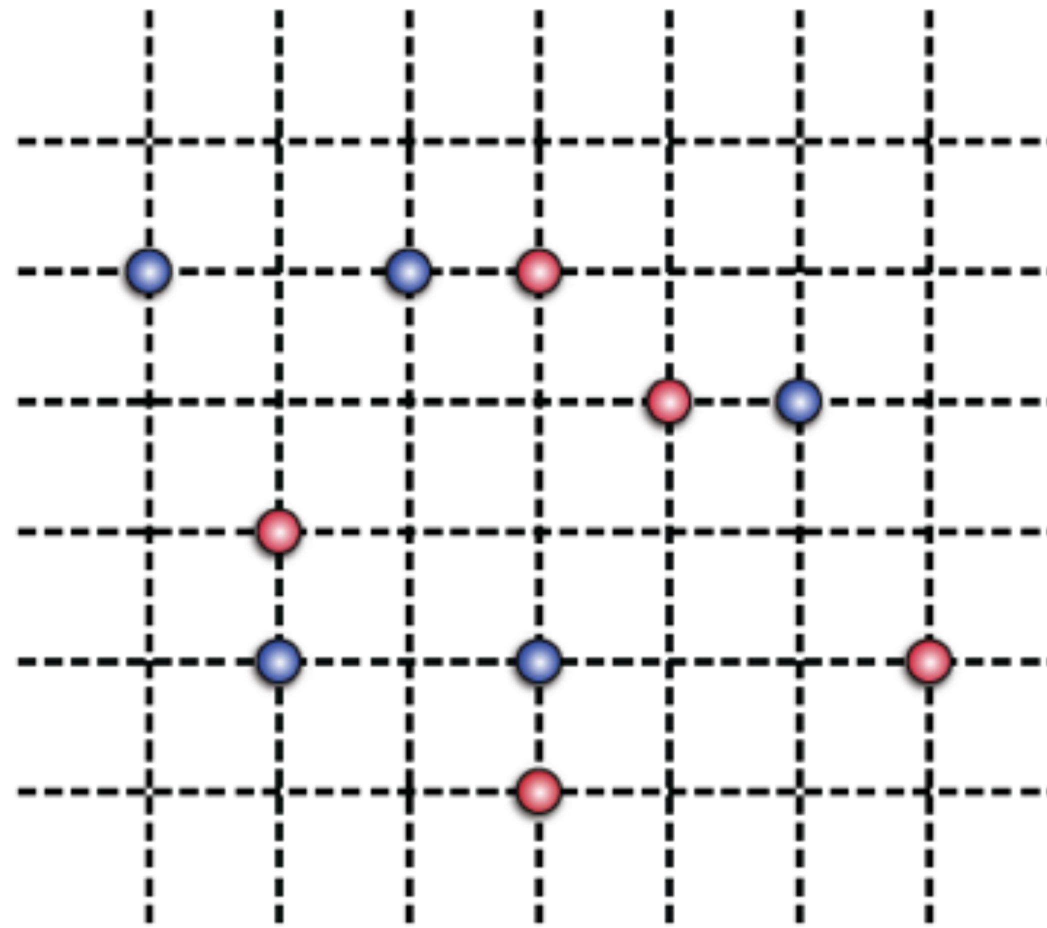

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Bosonic term
(k-point correlation function)

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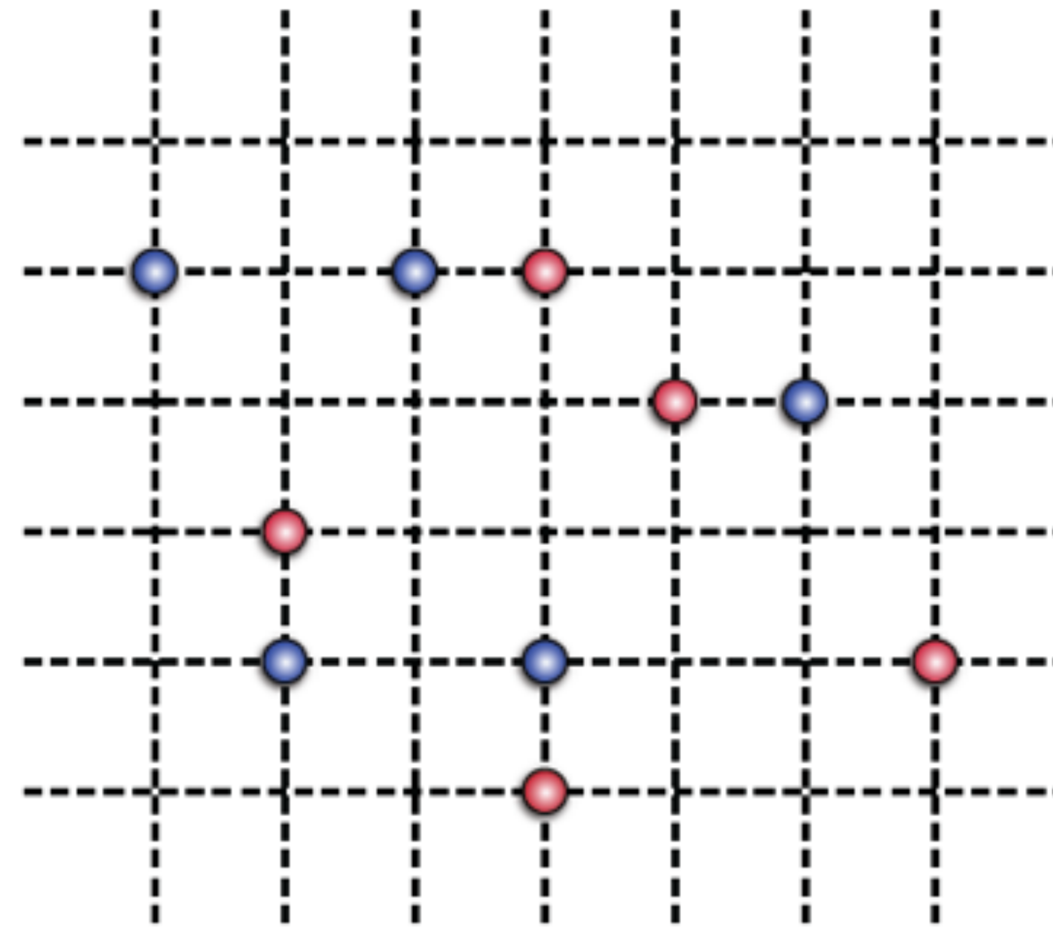

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$$\left\{ \int [\mathbf{d}\overline{\psi}\mathbf{d}\psi]\ \mathrm{e}^{-\overline{\psi}\ \mathbf{D^0}\ \psi}\ \overline{\psi}_{\mathbf{z_1}}\psi_{\mathbf{z_1}} \ldots \overline{\psi}_{\mathbf{z_k}}\psi_{\mathbf{z_k}} \right\}$$

Bosonic term
(k-point correlation function)

Fermionic term
(k-point correlation function)

Concept of Fermion Bags

Concept of Fermion Bags

S.C. Lattice 2008,2010
S.C, A.Li 2011,2012

Concept of Fermion Bags

S.C. Lattice 2008,2010

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Fermion k-point correlation function

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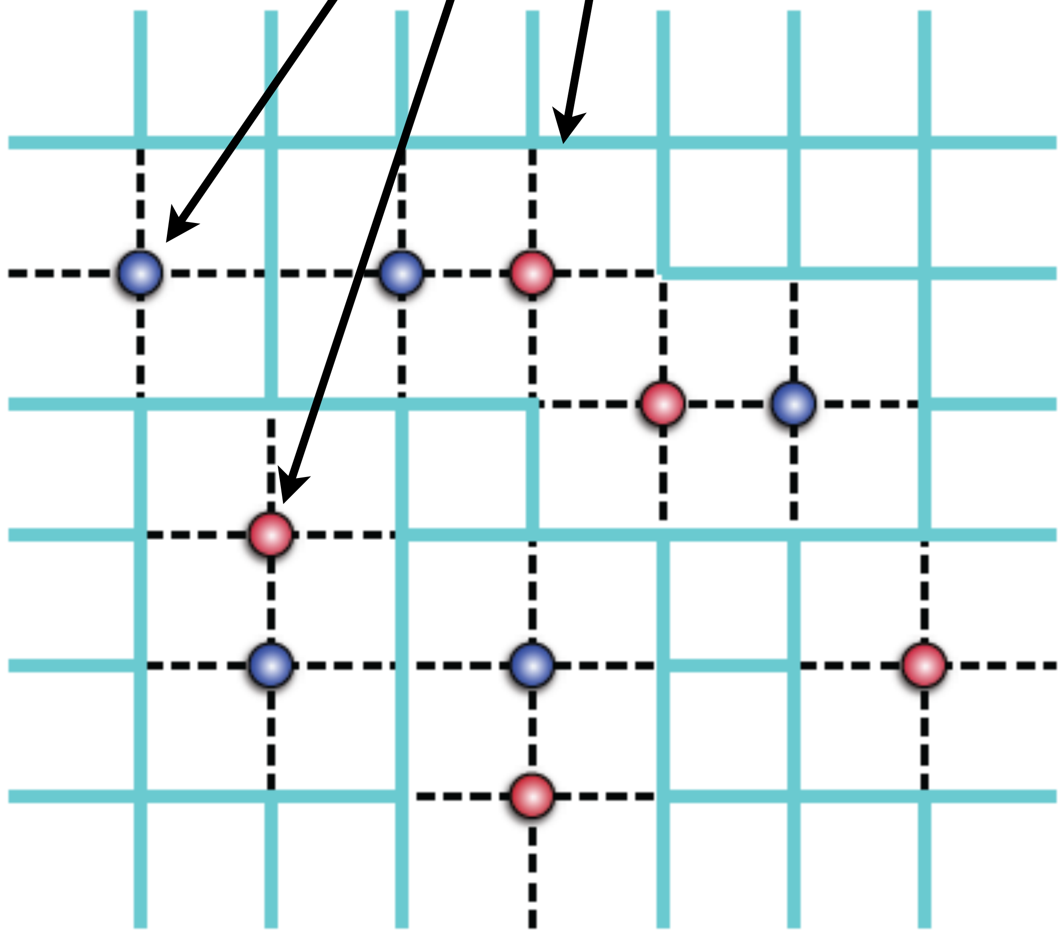
Fermion bags



fermion bag configuration

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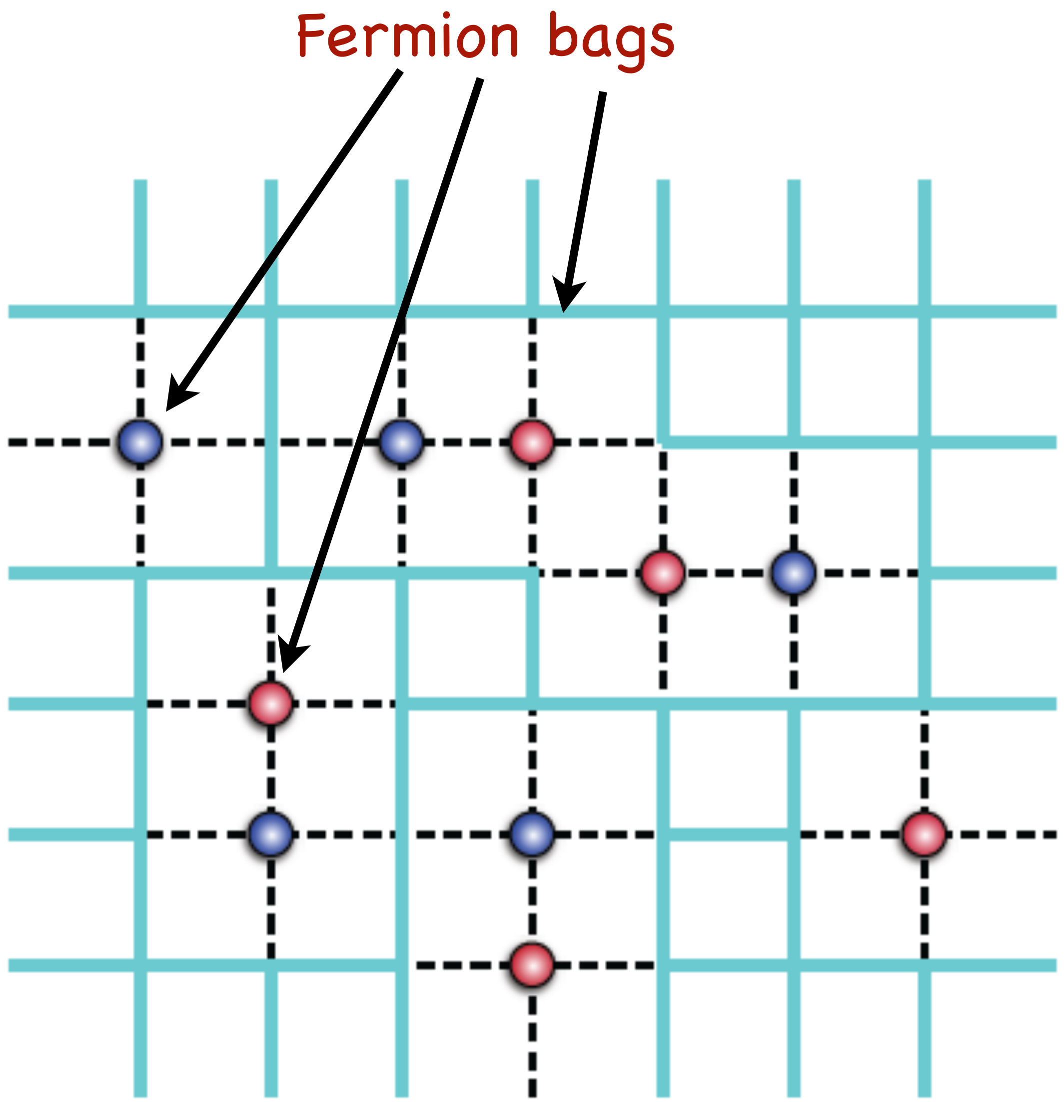
$$= \ \mathrm{Det}\Big(\mathbf{W^0}[\mathbf{n}]\Big)\ \geq \mathbf{0}$$



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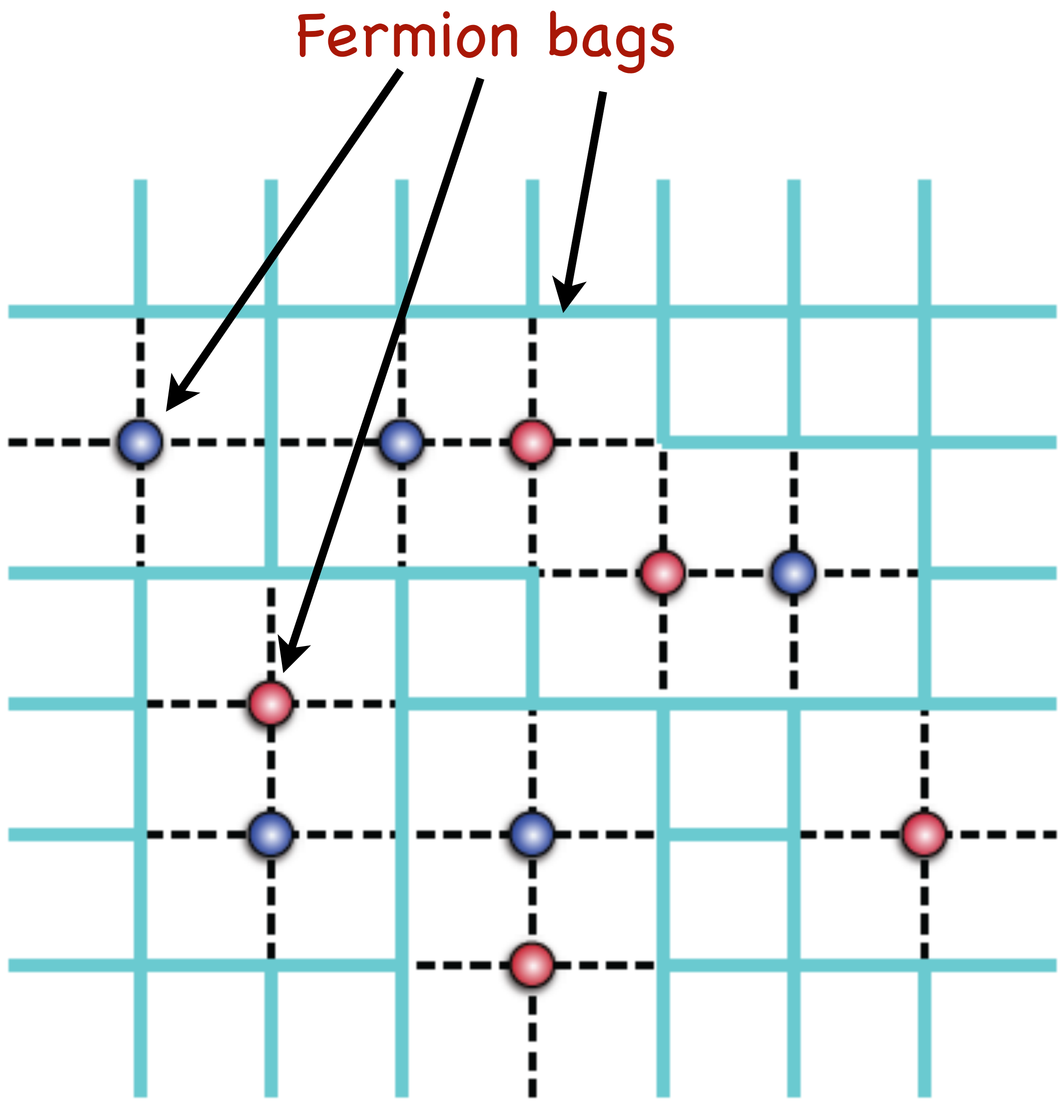

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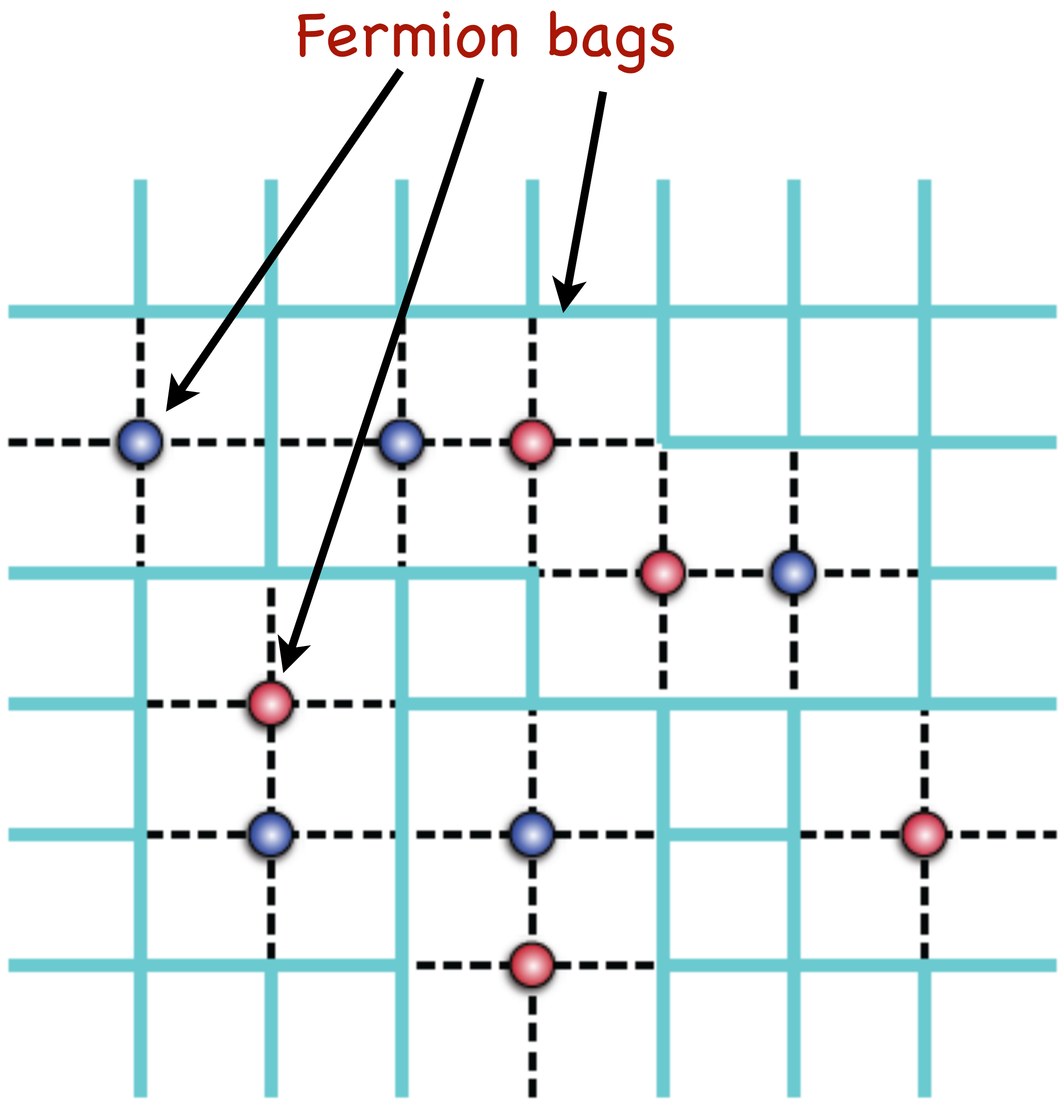

fermion bag configuration

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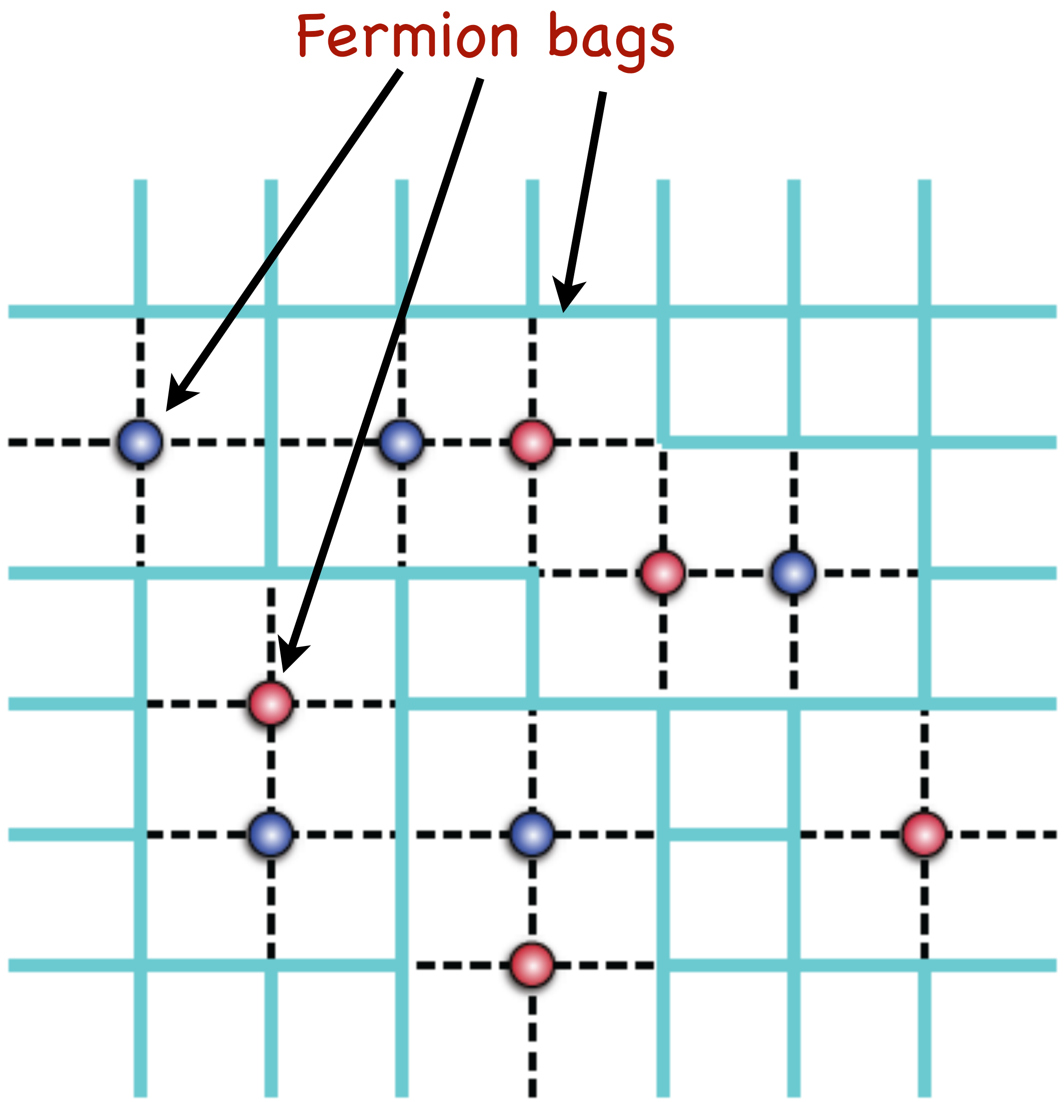
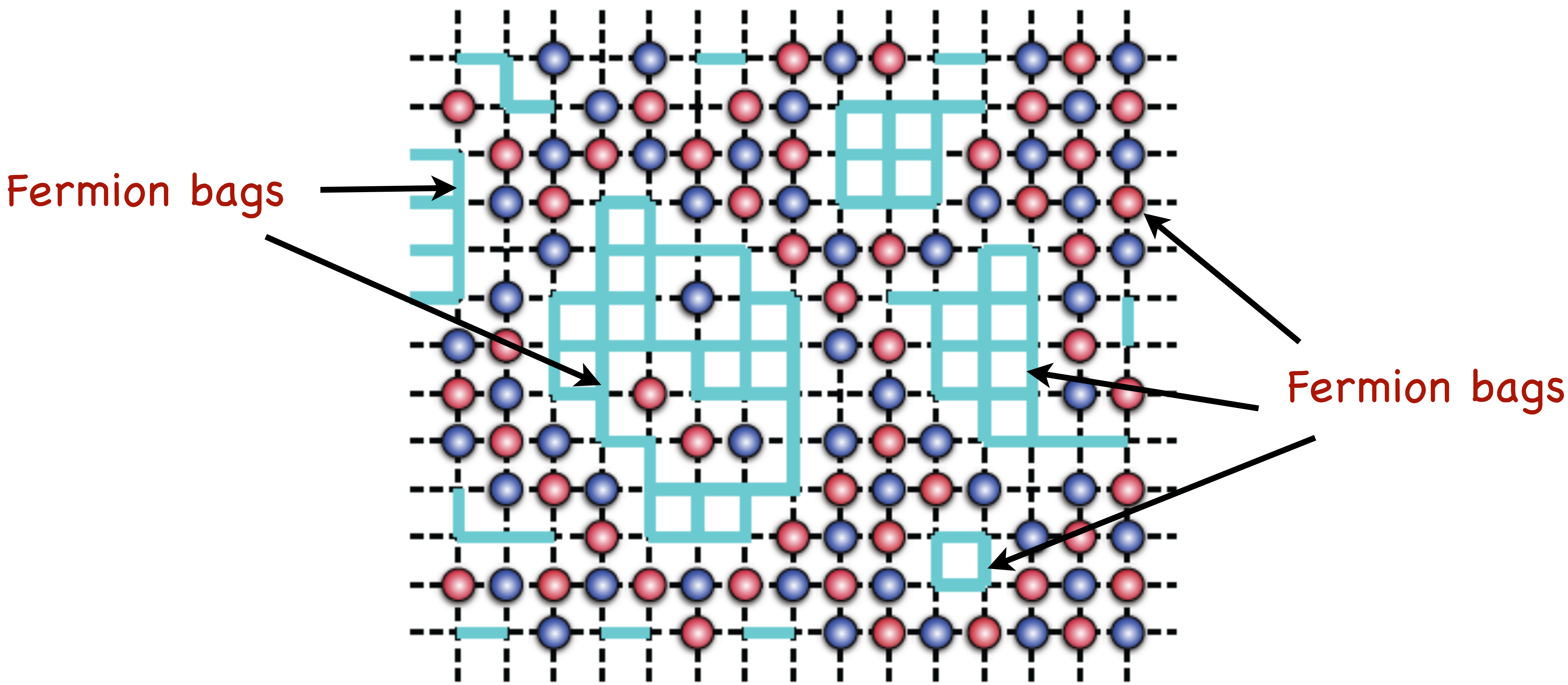


fermion bag configuration

Fermion Bags --> A collection of fermion d-o-f

At large coupling --> many small fermion bags

At large coupling --> many small fermion bags



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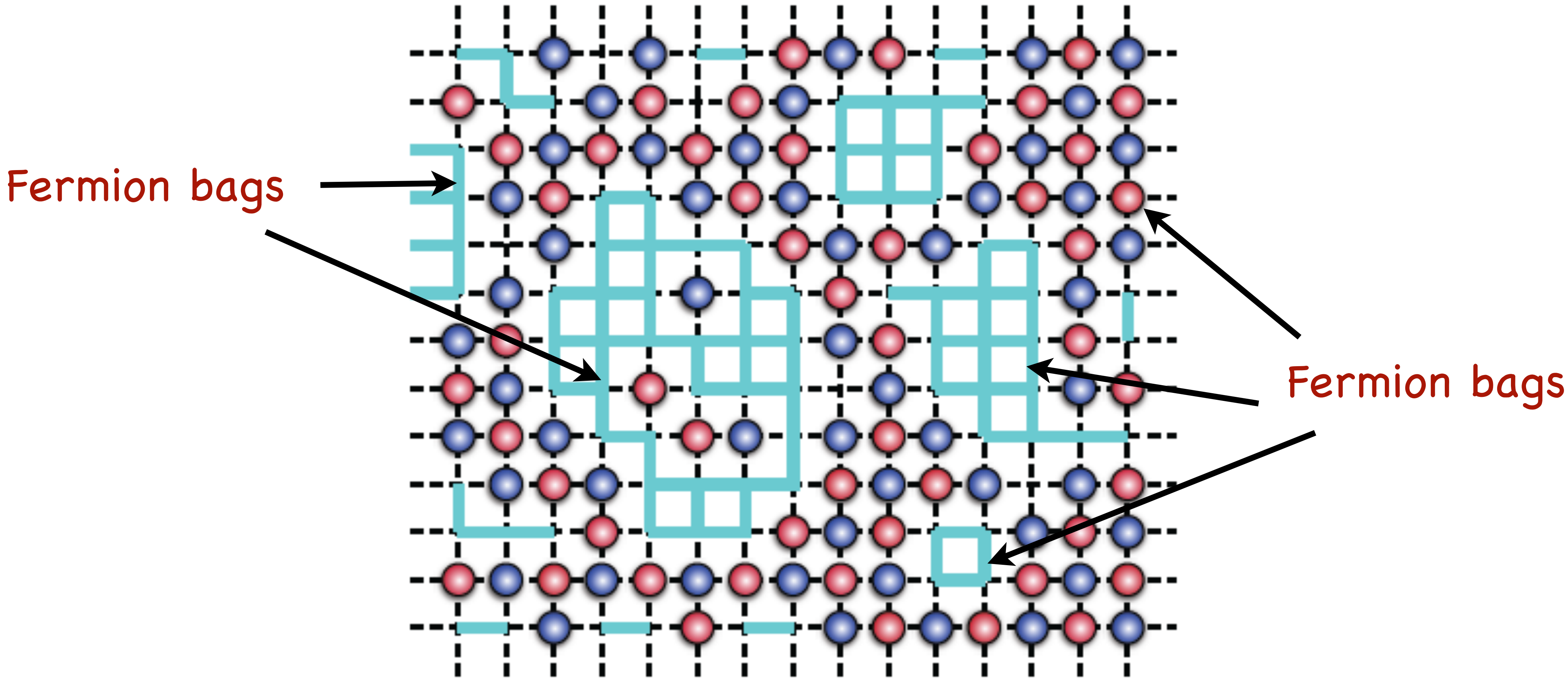

small fermion bags --> massive fermions

Connection to Determinantal Diagrammatic Monte Carlo

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

Connection to Determinantal Diagrammatic Monte Carlo

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k-point correlation function

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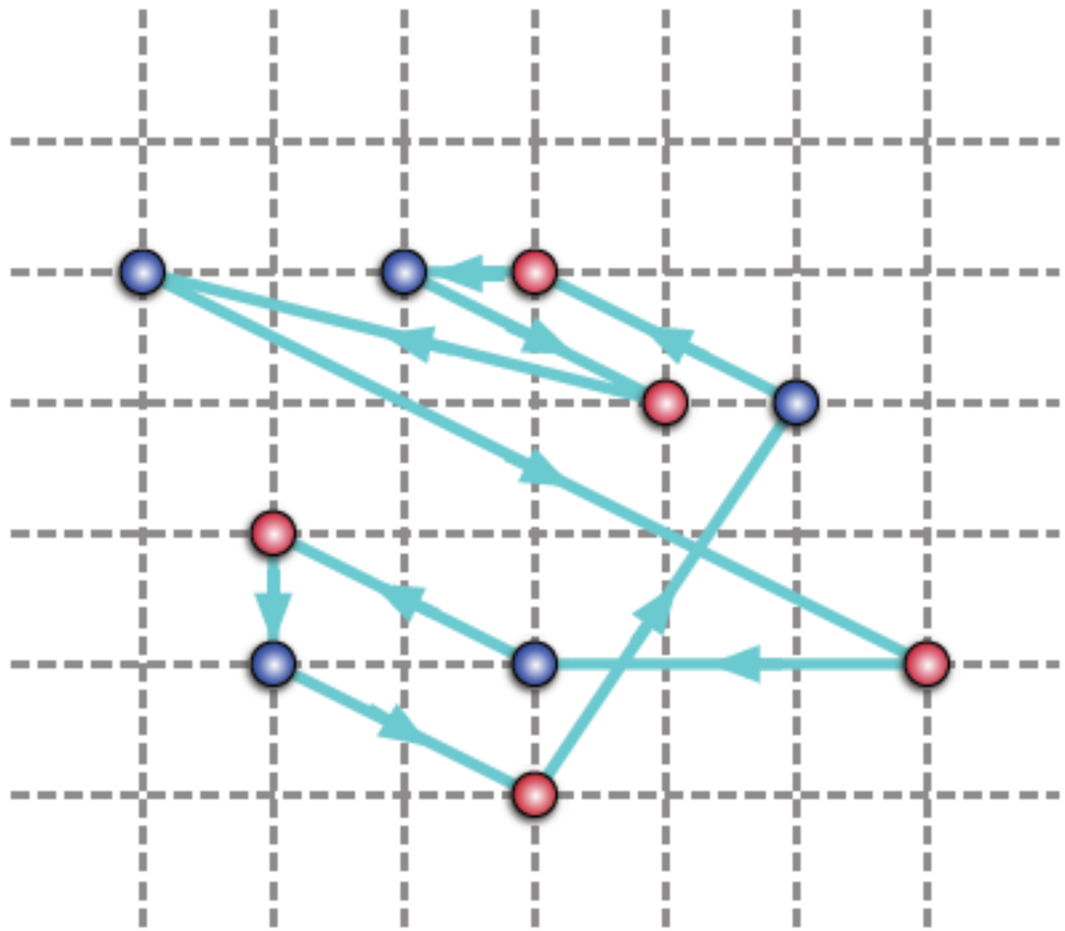

Dual Fermion Bag

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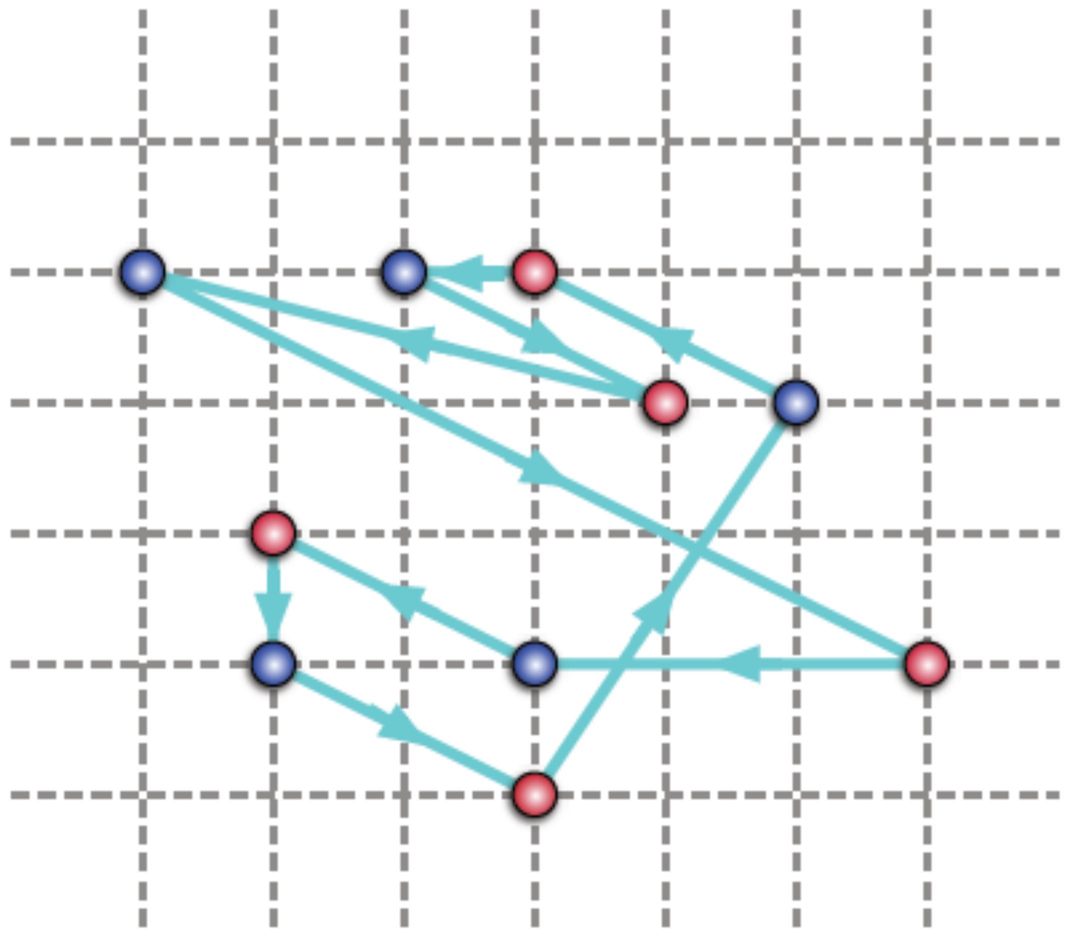

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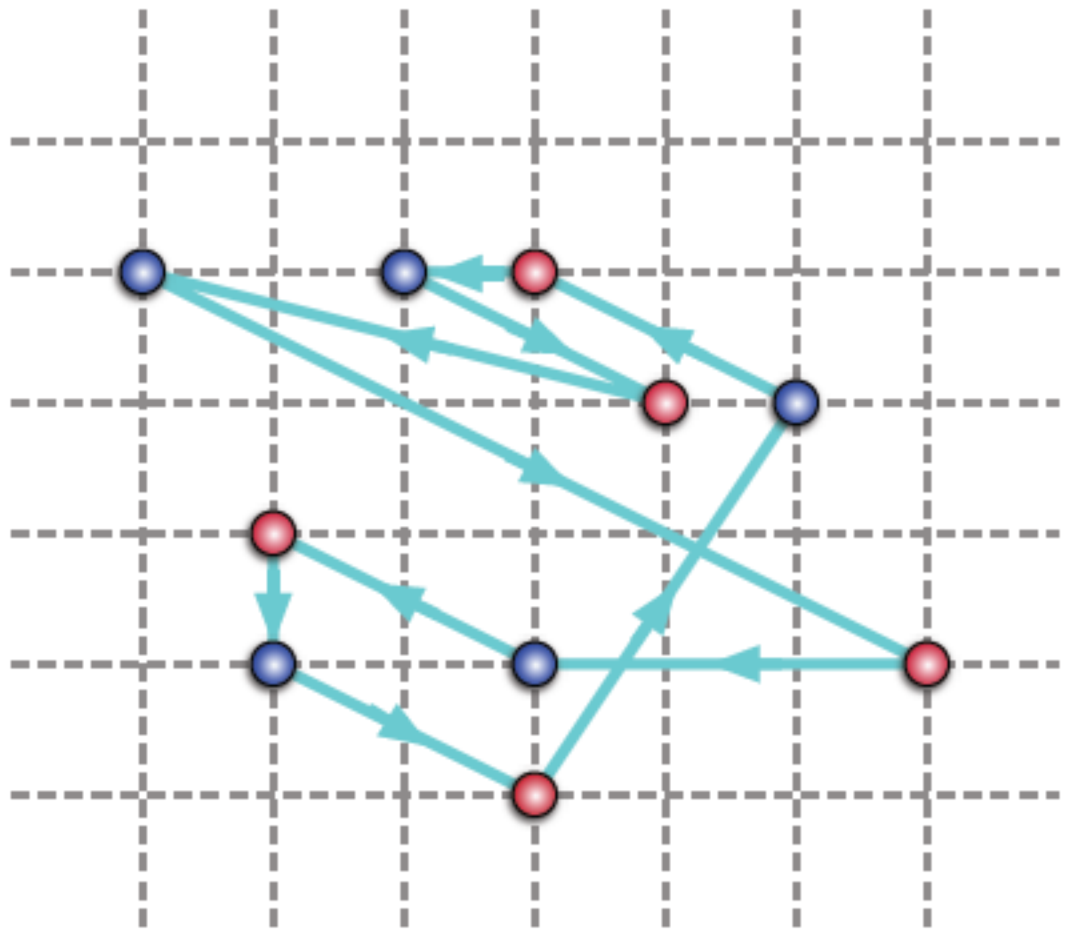
where $G_{[n]}$ is a (k x k) matrix of propagators



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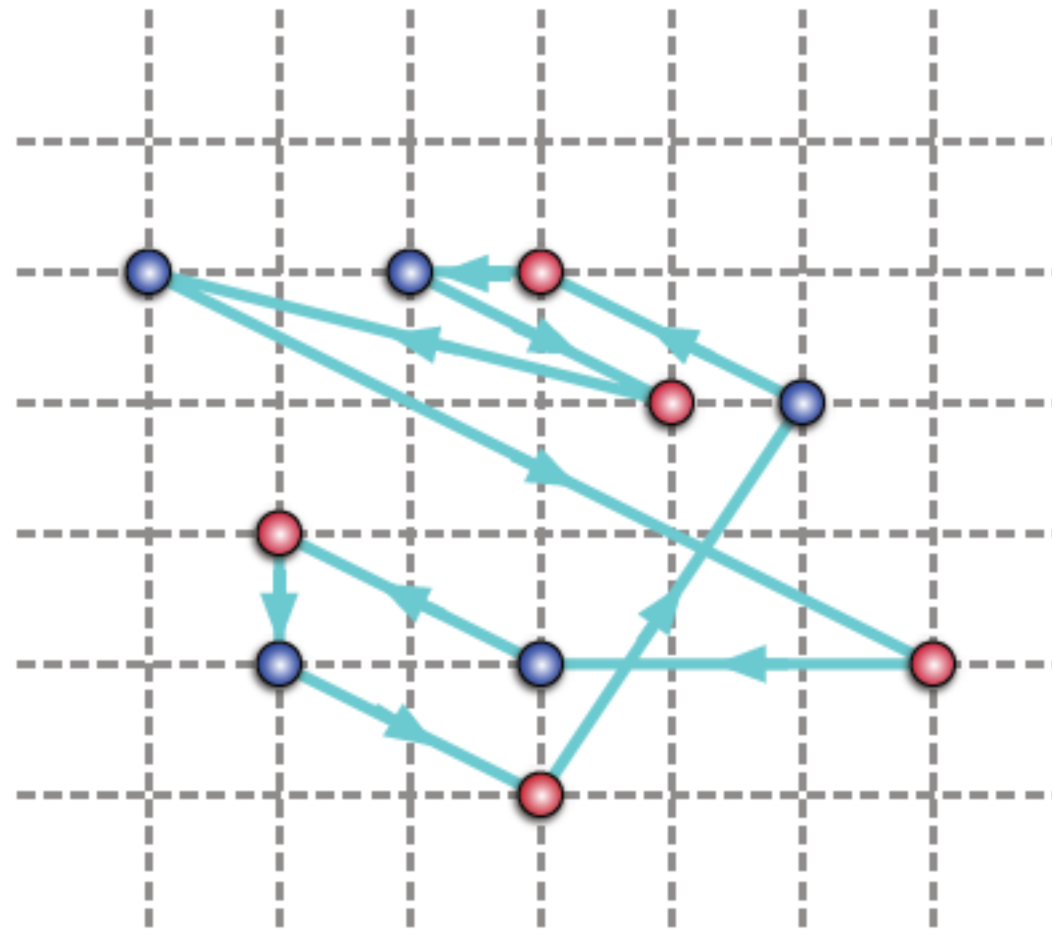

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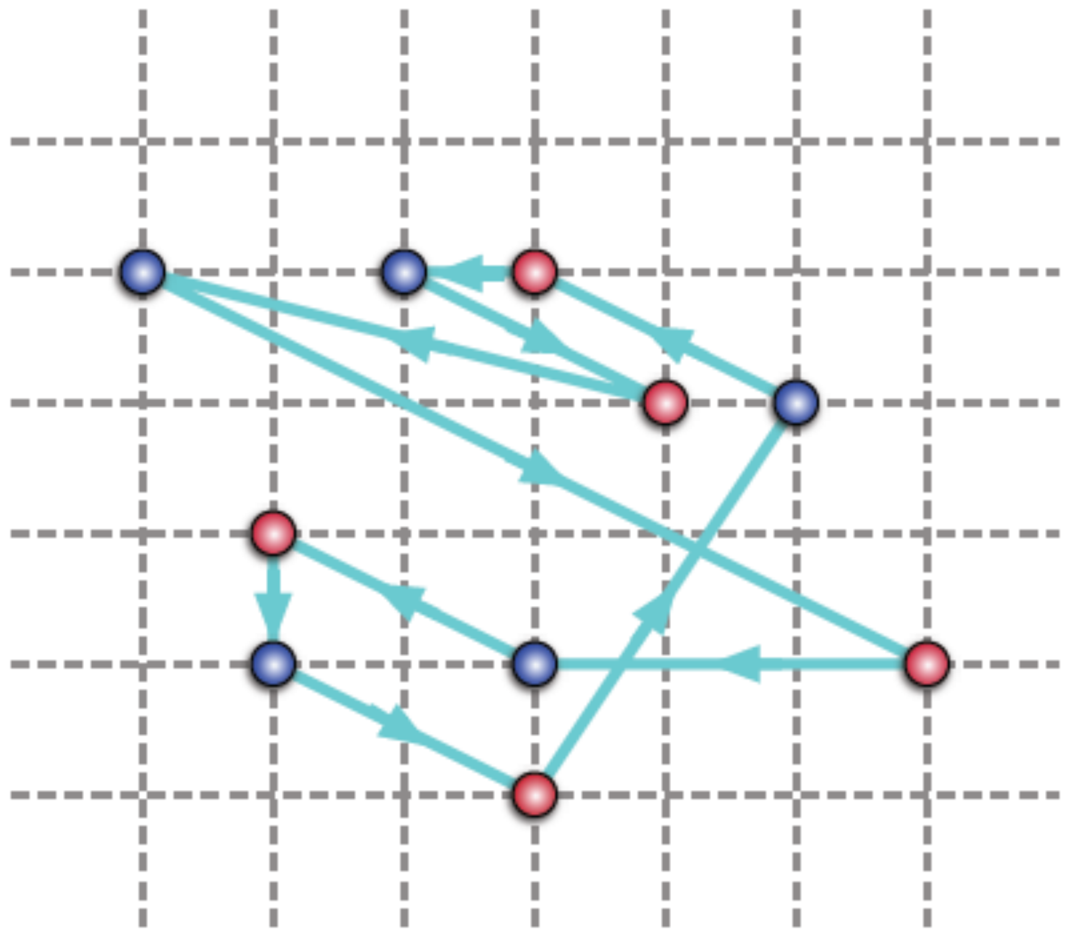

Dual Fermion Bag

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strong coupling fermion bag

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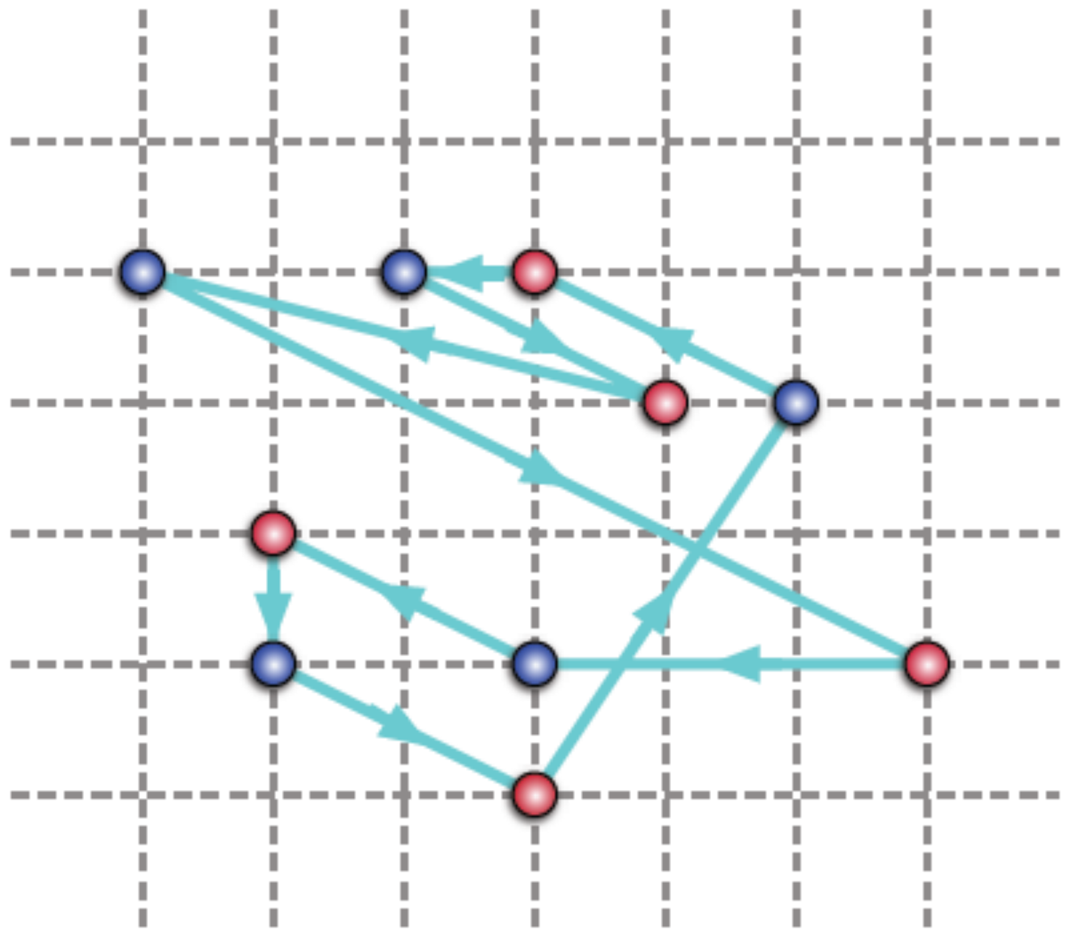

Dual Fermion Bag

Duality Relation

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

strong coupling fermion bag

weak coupling fermion Bag

What about the Bosonic k-point correlation function

What about the Bosonic k-point correlation function

Using the identity

$$e^{\beta\cos(\theta_{\mathbf{x}}-\theta_{\mathbf{x}+\alpha})} = \sum_{\mathbf{k}_{\mathbf{x},\alpha}} \mathbf{I}_{\mathbf{k}_{\mathbf{x},\alpha}}(\beta) e^{\mathbf{i}(\theta_{\mathbf{x}}-\theta_{\mathbf{x}+\alpha})}$$

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can show D.Banerjee, S.C PRD(2010)

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can show D.Banerjee, S.C PRD(2010)

$$\int[\mathbf{d}\theta]\Bigg(\prod_{\langle\mathbf{x},\alpha\rangle}\mathrm{e}^{\beta\cos(\theta_{\mathbf{x}}-\theta_{\mathbf{x}+\alpha})}$$

$$\mathrm{e}^{\mathbf{i}\varepsilon_{\mathbf{z_1}}\theta_{\mathbf{z_1}}}\mathrm{e}^{\mathbf{i}\varepsilon_{\mathbf{z_2}}\theta_{\mathbf{z_2}}}\ldots\mathrm{e}^{\mathbf{i}\varepsilon_{\mathbf{z_k}}\theta_{\mathbf{z_k}}}\Bigg)$$

$$=\sum_{[\mathbf{k}]}\Bigg(\prod_{\langle\mathbf{x},\alpha\rangle}\mathbf{I}_{\mathbf{k}_{\mathbf{x},\alpha}}\Bigg)$$

$$\Bigg\{\prod_{\mathbf{x}}\delta\Big(\varepsilon_{\mathbf{x}}\mathbf{n}_{\mathbf{x}}+\sum_{\alpha}(\mathbf{k}_{\mathbf{x},\alpha}-\mathbf{k}_{\mathbf{x}-\alpha,\alpha})\Big)\Bigg\}$$

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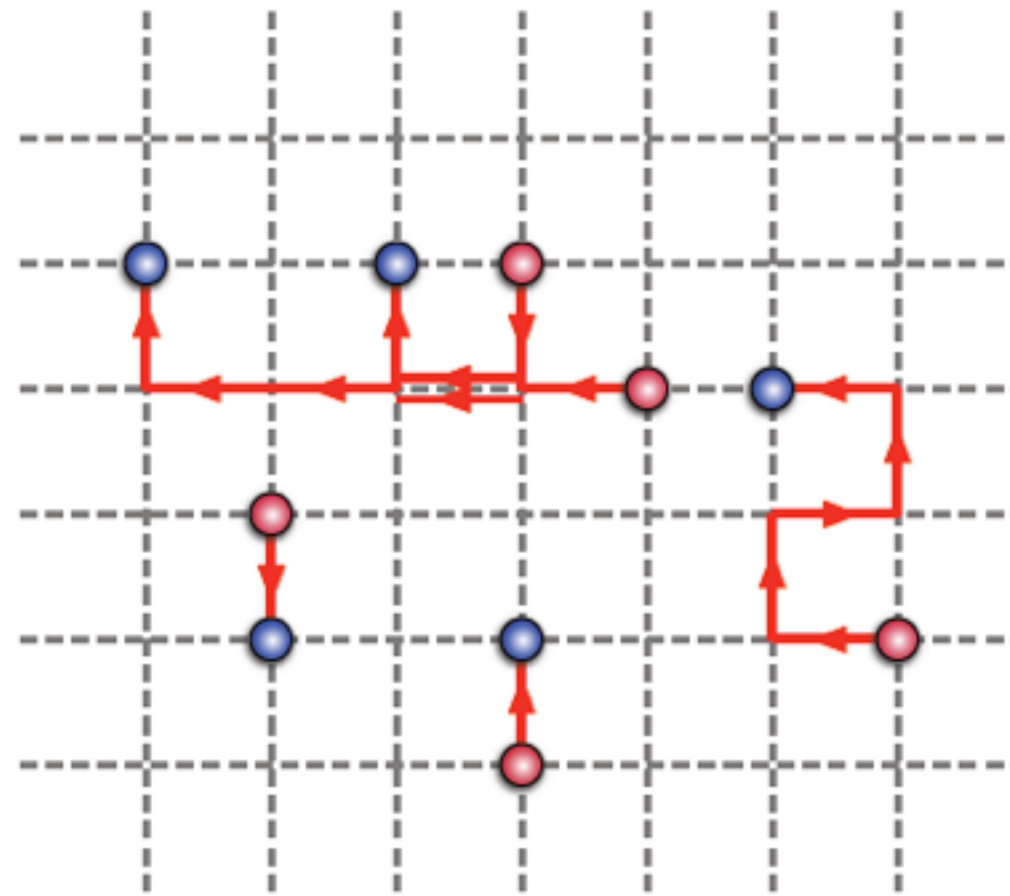
can show D.Banerjee, S.C PRD(2010)

$$\int [\mathbf{d}\theta] \Bigg(\prod_{\langle \mathbf{x},\alpha\rangle} e^{\beta\cos(\theta_{\mathbf{x}}-\theta_{\mathbf{x}+\alpha})} e^{\mathbf{i}\varepsilon_{\mathbf{z_1}}\theta_{\mathbf{z_1}}} e^{\mathbf{i}\varepsilon_{\mathbf{z_2}}\theta_{\mathbf{z_2}}} \ldots e^{\mathbf{i}\varepsilon_{\mathbf{z_k}}\theta_{\mathbf{z_k}}} \Bigg)$$

$$= \sum_{[\mathbf{k}]} \Bigg(\prod_{\langle \mathbf{x},\alpha\rangle} \mathbf{I}_{\mathbf{k}_{\mathbf{x},\alpha}} \Bigg) \Bigg\{ \prod_{\mathbf{x}} \delta\Big(\varepsilon_{\mathbf{x}}\mathbf{n}_{\mathbf{x}} + \sum_{\alpha} (\mathbf{k}_{\mathbf{x},\alpha} - \mathbf{k}_{\mathbf{x}-\alpha,\alpha})\Big) \Bigg\}$$



example of a [k] configuration consistent with [n]

Thus, the partition function is given by

$$\mathbf{Z} = \sum_{[\mathbf{n},\mathbf{k}]} \mathbf{g}^{\mathbf{k}} \mathrm{Det}\Big(\mathbf{W^0}[\mathbf{n}]\Big) \Big(\prod_{\mathbf{x},\alpha} \mathbf{I}_{\mathbf{k}_{\mathbf{x},\alpha}}\Big)$$

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No sign problem!

Thus, the partition function is given by

$$\mathbf{Z} = \sum_{[\mathbf{n},\mathbf{k}]} \mathbf{g}^{\mathbf{k}} \mathrm{Det}\Big(\mathbf{W}^{\mathbf{0}}[\mathbf{n}]\Big) \Big(\prod_{\mathbf{x},\alpha} \mathbf{I}_{\mathbf{k}_{\mathbf{x},\alpha}}\Big)$$

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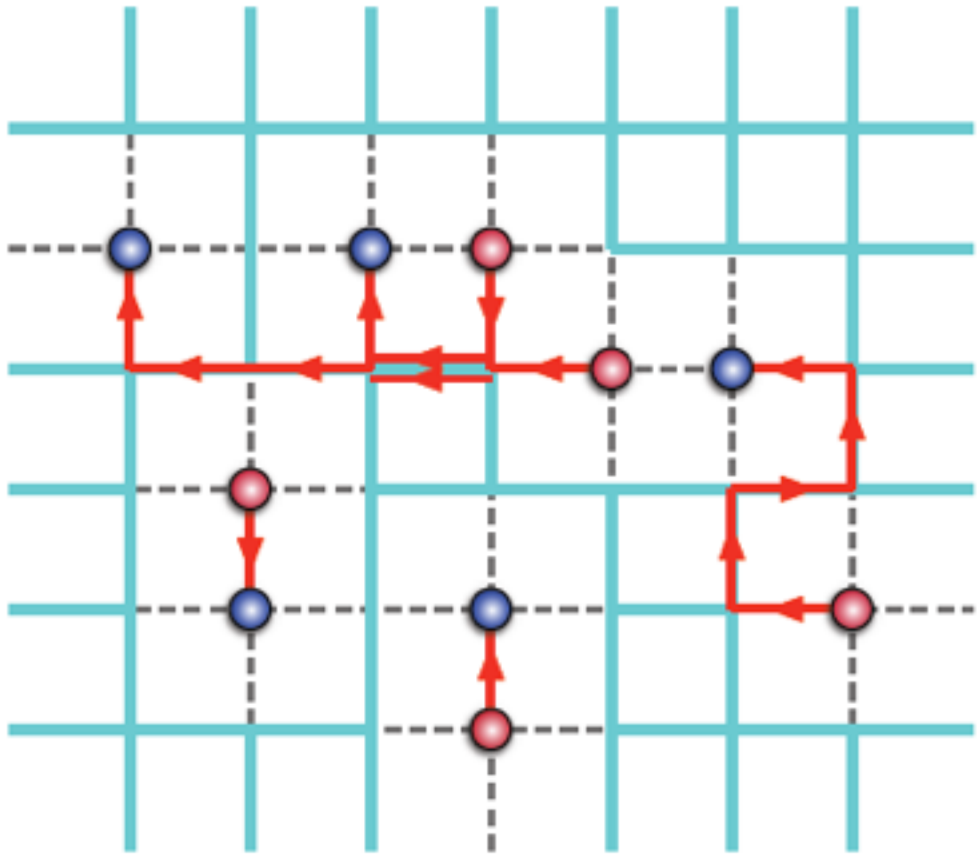

[n,k] configurations

Applications?

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3d Thirring and Gross-Neveu Models

Lattice Thirring Model

Lattice Thirring Model

Barbour, Debbio, Focht, Hands, Lucini, Strouthos,...

Lattice Thirring Model

Barbour, Debbio, Focht, Hands, Lucini, Strouthos,...

$$S_T = \frac{1}{2}\sum_{x,\alpha} \eta_{x,\alpha}\left\{\overline{\psi}_x(1+g\ \mathrm{e}^{i\theta_{x,\alpha}})\psi_{x+\alpha} - \overline{\psi}_{x+\alpha}(1+g\ \mathrm{e}^{-i\theta_{x,\alpha}})\psi_x\right\}$$

$$+\, m \sum_x \overline{\psi}_x\psi_x$$

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auxiliary gauge field

auxiliary gauge field

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Symmetry : SU(2) x U(1)

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No sign problem in traditional MC method

But can be solved also in the fermion bag approach!

Lattice Gross-Neveu Model

Lattice Gross-Neveu Model

Christofi, Hands, Karkkainen, Kocic, Kogut, Strouthos,...

Lattice Gross-Neveu Model

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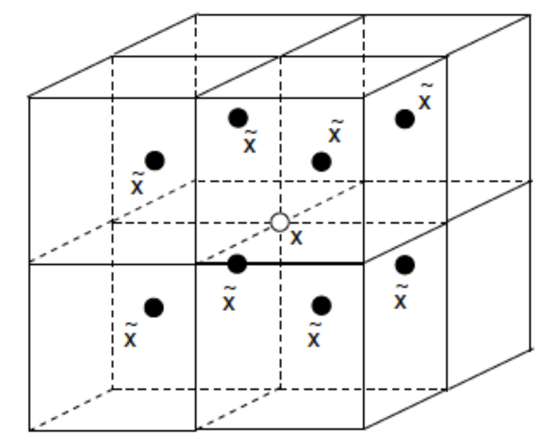

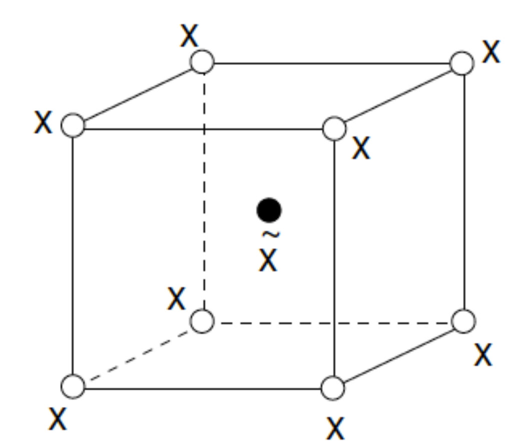

Lattice Gross-Neveu Model

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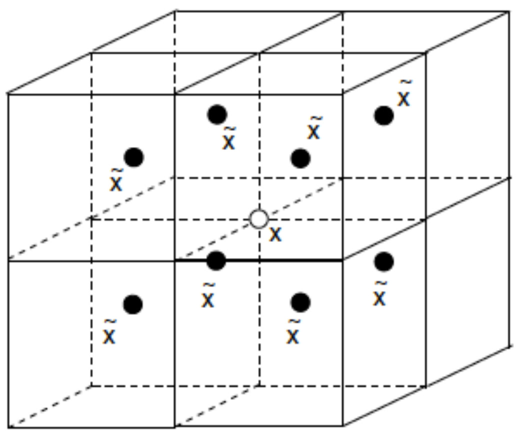
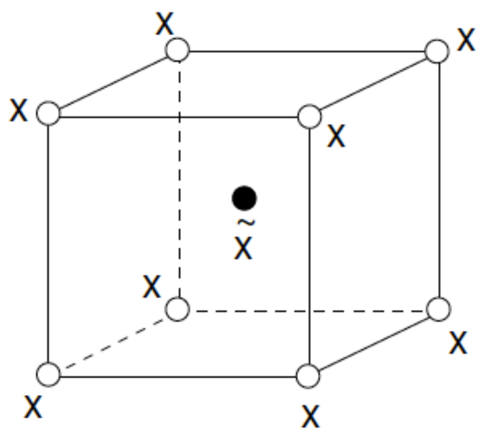
$$S_{GN} = \sum_{x,y} \overline{\psi}_x \left\{ D^0_{xy} \; + \; \delta_{xy} \overline{\phi}_x \right\} \psi_y \quad + \quad S_b[\sigma_{\tilde{x}}, \pi_{\tilde{x}}]$$





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$$S_{GN} = \sum_{x,y} \overline{\psi}_x \left\{ D^0_{xy} + \delta_{xy}\overline{\phi}_x \right\} \psi_y + S_b[\sigma_{\tilde{x}}, \pi_{\tilde{x}}]$$

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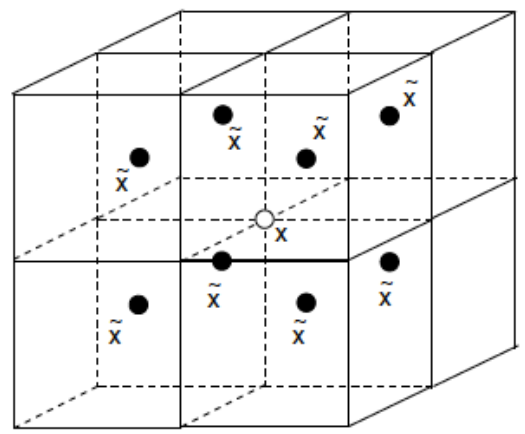

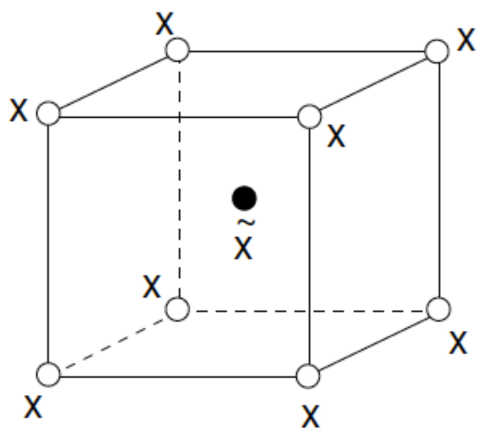

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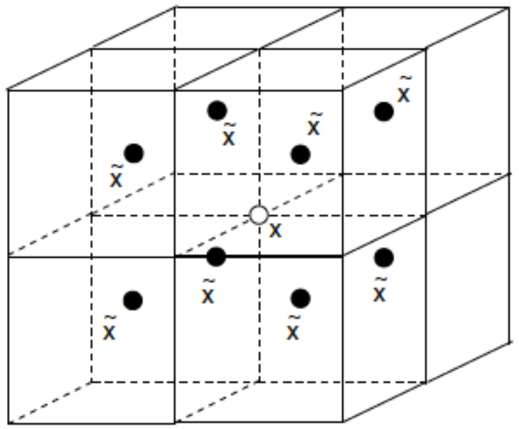

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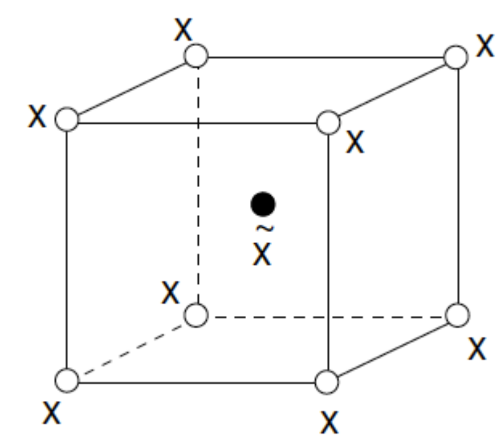

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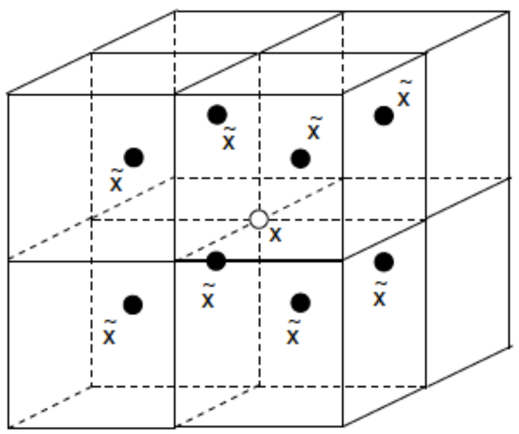
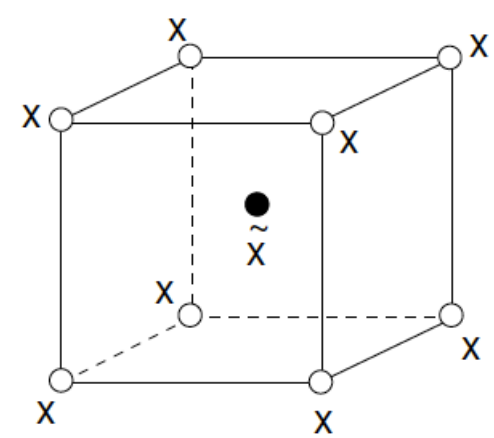
$$S_b[\sigma_{\tilde{x}}, \pi_{\tilde{x}}] = \frac{1}{4g^2} \sum_{\tilde{x}} \left[(\sigma_{\tilde{x}})^2 + (\pi_{\tilde{x}})^2 \right]$$

$$\overline{\phi}_x = \frac{1}{8} \sum_{\tilde{x}} (\sigma_{\tilde{x}} + i\varepsilon_x \pi_{\tilde{x}})$$





Symmetry: SU(2) x U(1)

Lattice Gross-Neveu Model

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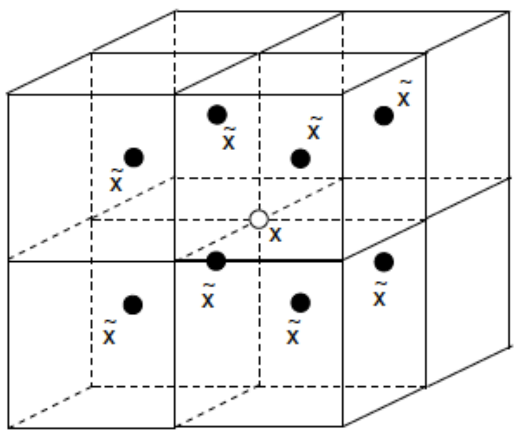

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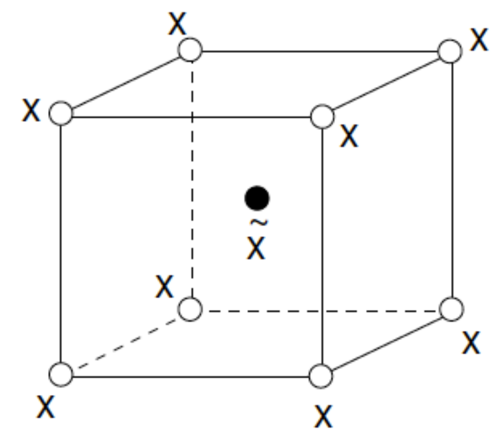

Symmetry: SU(2) x U(1)

Suffers from sign problem
in the traditional method
but not in the fermion bag approach!

Fermion Bag Approach

Fermion Bag Approach

S.C. A.Li PRL (2012)

Fermion Bag Approach

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$$\mathbf{S}(\theta,\overline{\psi},\psi) = \sum_{\mathbf{xy}} \overline{\psi}_{\mathbf{x}} \mathbf{D}^{\mathbf{0}}_{\mathbf{xy}} \psi_{\mathbf{x}} \; - \; \sum_{\langle \mathbf{xy} \rangle} \mathbf{U}_{\langle \mathbf{xy} \rangle} \overline{\psi}_{\mathbf{x}} \psi_{\mathbf{x}} \; \overline{\psi}_{\mathbf{y}} \psi_{\mathbf{y}}$$

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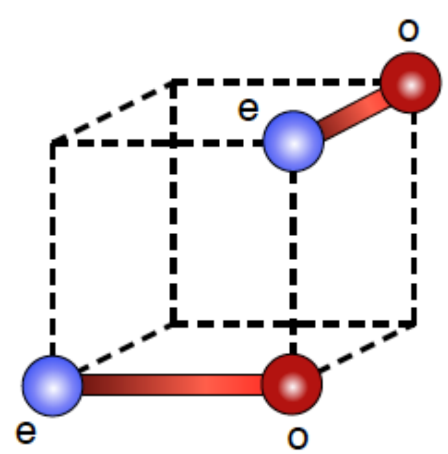

Thirring

Fermion Bag Approach

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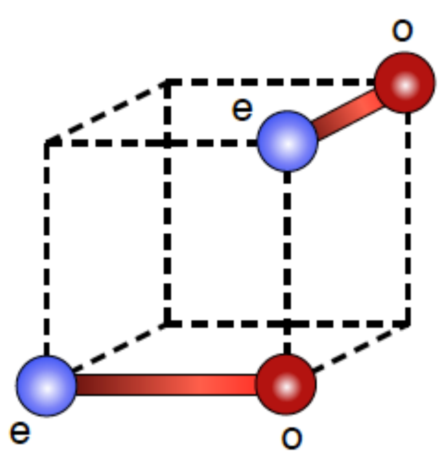
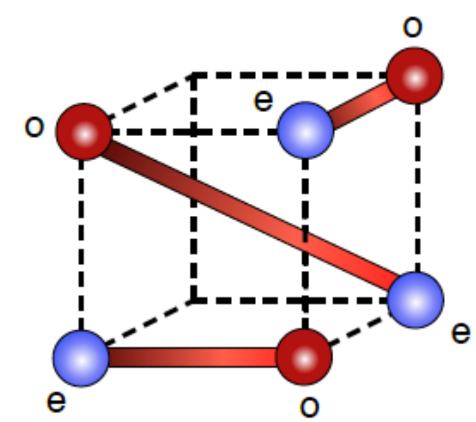


Thirring



Gross-Neveu

Fermion Bag Approach

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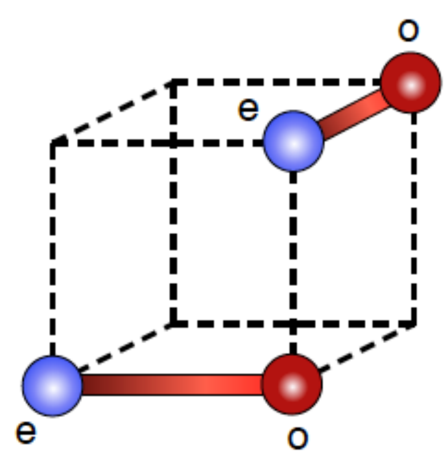
$$\mathbf{S}(\theta,\overline{\psi},\psi) = \sum_{\mathbf{xy}} \overline{\psi}_{\mathbf{x}} \mathbf{D}^{\mathbf{0}}_{\mathbf{xy}} \psi_{\mathbf{x}} \;-\; \sum_{\langle \mathbf{xy}\rangle} \mathbf{U}_{\langle \mathbf{xy}\rangle} \overline{\psi}_{\mathbf{x}} \psi_{\mathbf{x}}\; \overline{\psi}_{\mathbf{y}} \psi_{\mathbf{y}}$$



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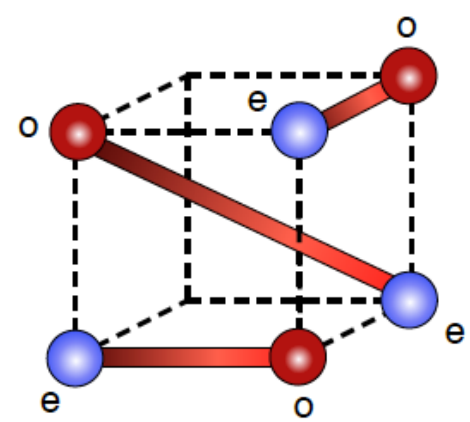
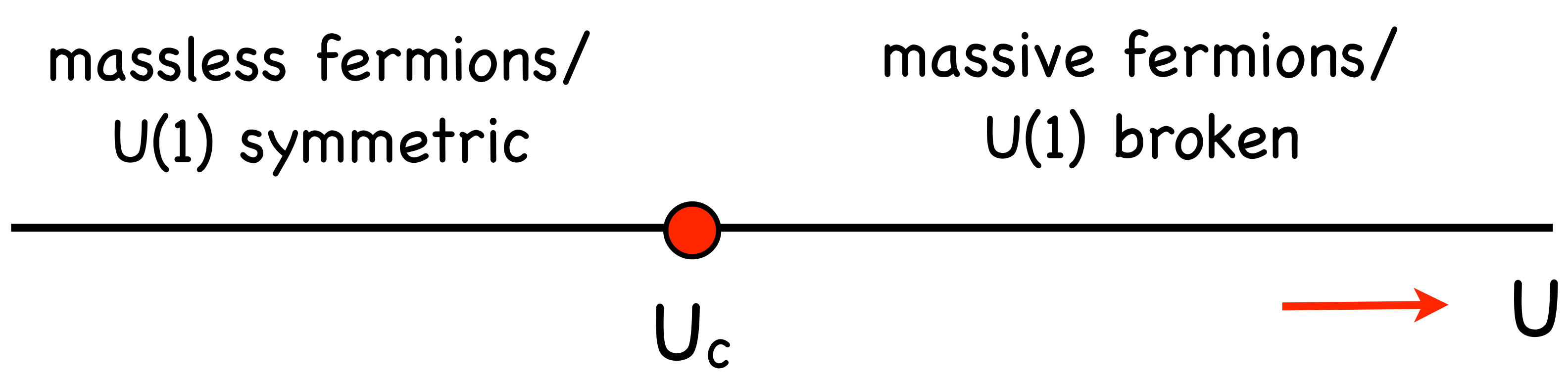


Gross-Neveu



partition function

partition function

strong coupling

$$\mathbf{Z} = \sum_{[\mathbf{b}]} \mathbf{U}^{\mathbf{k}} \, \mathrm{Det}\Big(\mathbf{W}^{\mathbf{0}}[\mathbf{b}]\Big)$$

(V-k) x (V-k) matrix

partition function

strong coupling

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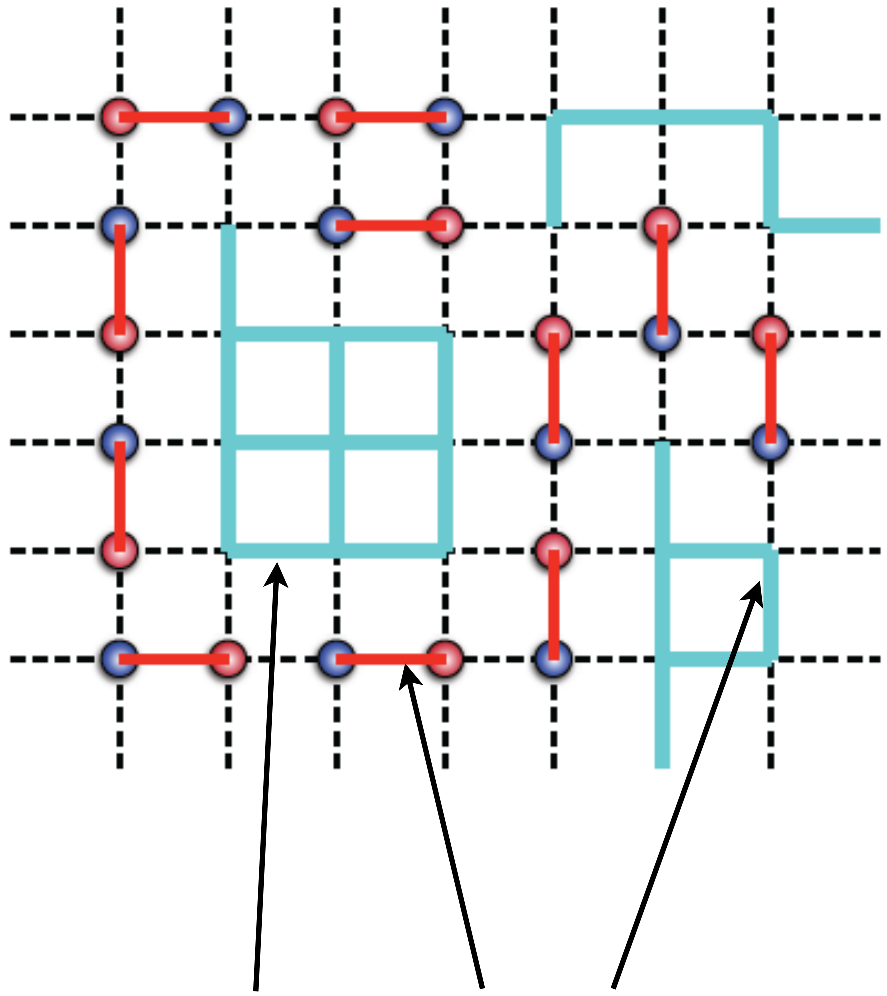


fermion bags

partition function

strong coupling

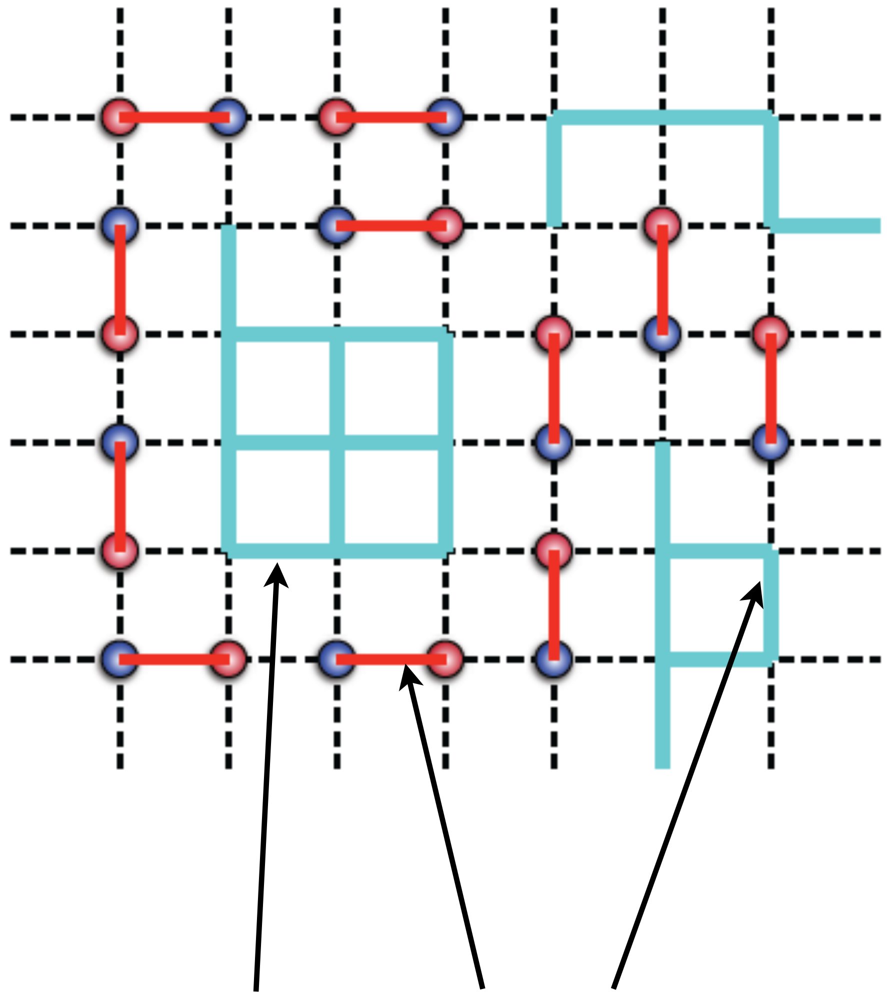
$$\mathbf{Z} = \sum_{[\mathbf{b}]} \mathbf{U}^{\mathbf{k}}\ \mathrm{Det}\left(\mathbf{W}^{\mathbf{0}}[\mathbf{b}]\right)$$

(V-k) x (V-k) matrix

weak coupling

$$\mathbf{Z} = \mathrm{Det}\left(\mathbf{D}^{\mathbf{0}}\right) \sum_{[\mathbf{b}]} \mathbf{U}^{\mathbf{k}}\ \mathrm{Det}\left(\mathbf{G}[\mathbf{b}]\right)$$

k x k matrix



fermion bags

Observables

Observables

chiral susceptibility

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

Observables

chiral susceptibility

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chiral winding susceptibility

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

Observables

chiral susceptibility

$$\chi = \left\langle \frac{1}{2L^3} \sum_{x,y} \overline{\psi}_x \psi_x \, \overline{\psi}_y \psi_y \right\rangle$$

chiral winding susceptibility

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

fermion correlation ratio

$$C_F(t) = \left\langle \frac{1}{3} \sum_\alpha \overline{\psi}_{0,0,0} \;\; \psi_{0,0,t\hat{\alpha}} \right\rangle$$

$$R_F \;=\; C_F(L/2-1)/C(1)$$

Critical Finite Size Scaling

Critical Finite Size Scaling

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

$$\langle \mathbf{q}_\chi^{\mathbf{2}} \rangle = \kappa_{\mathbf{0}} + \kappa_{\mathbf{1}}(\mathbf{U}-\mathbf{U_c})\mathbf{L}^{\mathbf{1}/\nu} + \kappa_{\mathbf{2}}(\mathbf{U}-\mathbf{U_c})^{\mathbf{2}}\mathbf{L}^{\mathbf{2}/\nu} + \ldots$$

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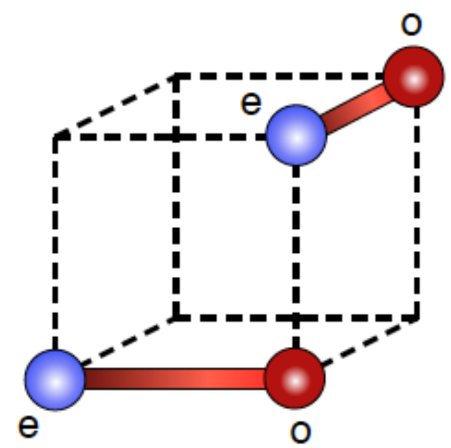
If we plot LHS w.r.t U
all quantities must be independent of L at $U = U_c$

Thirring model results

Thirring model results



Thirring

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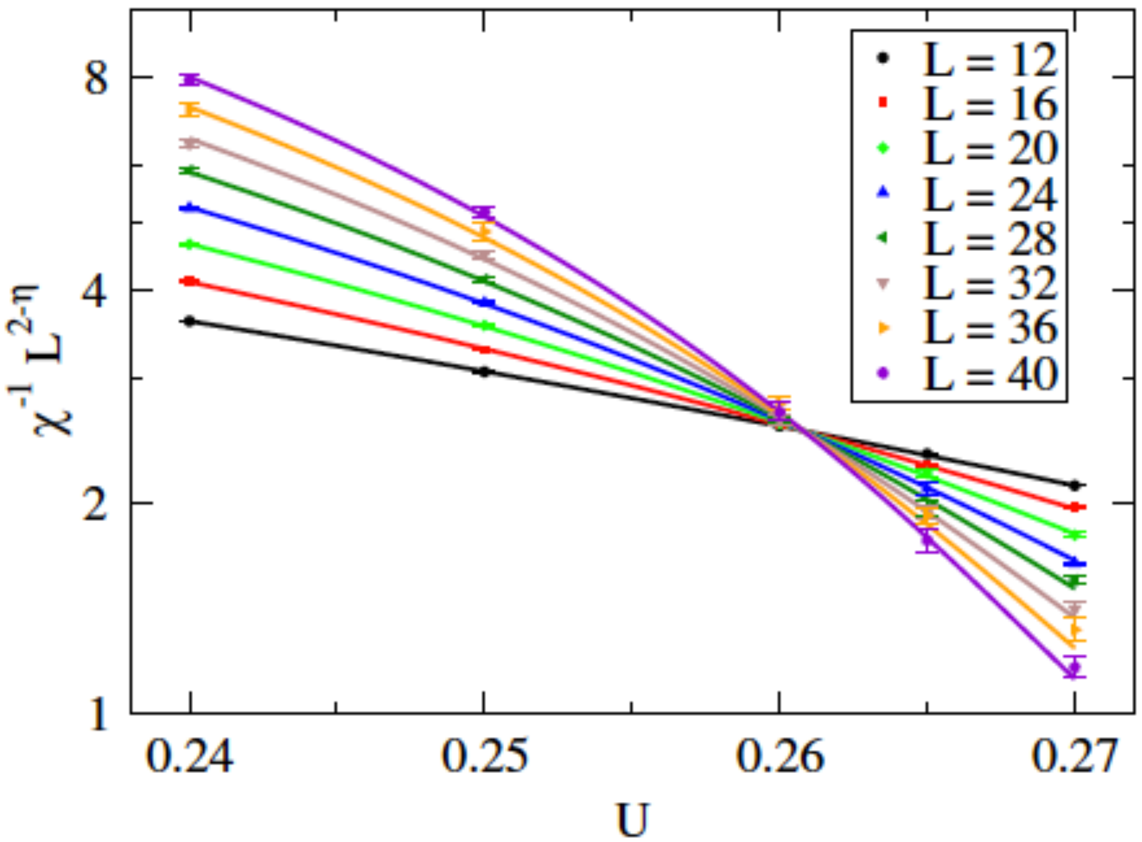

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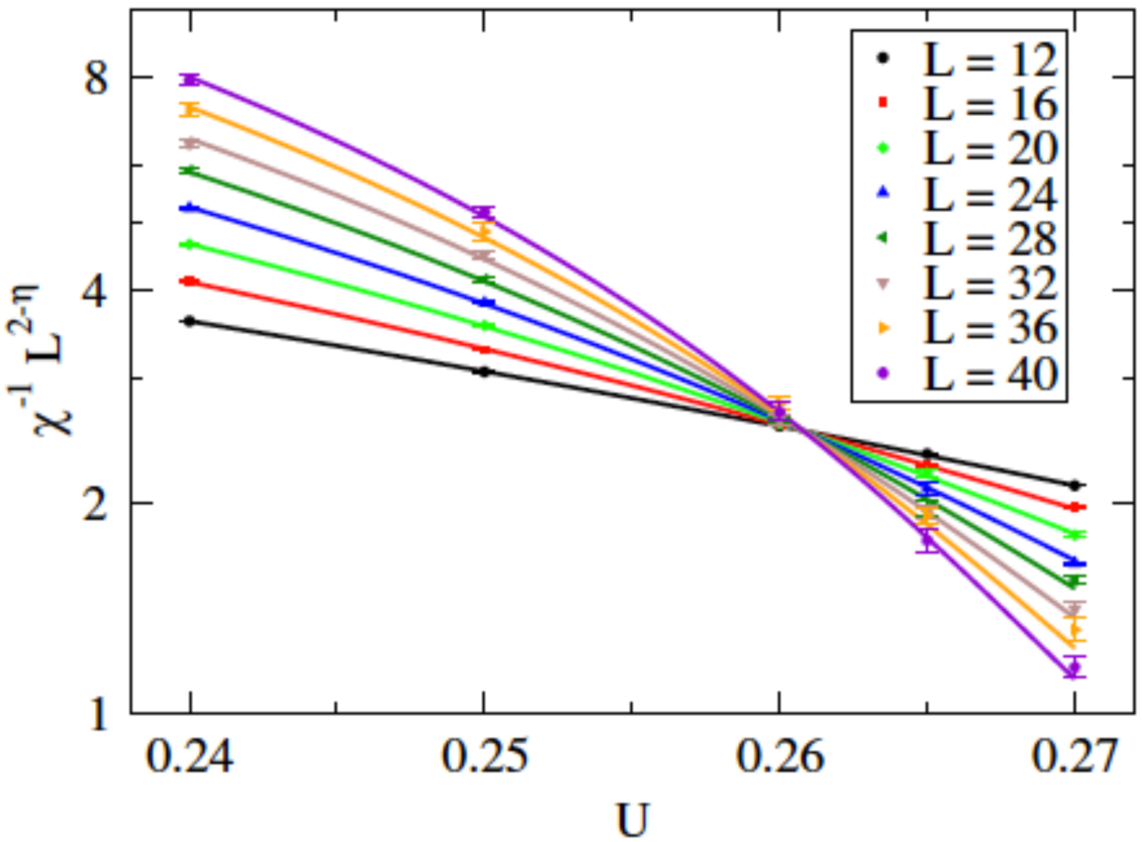

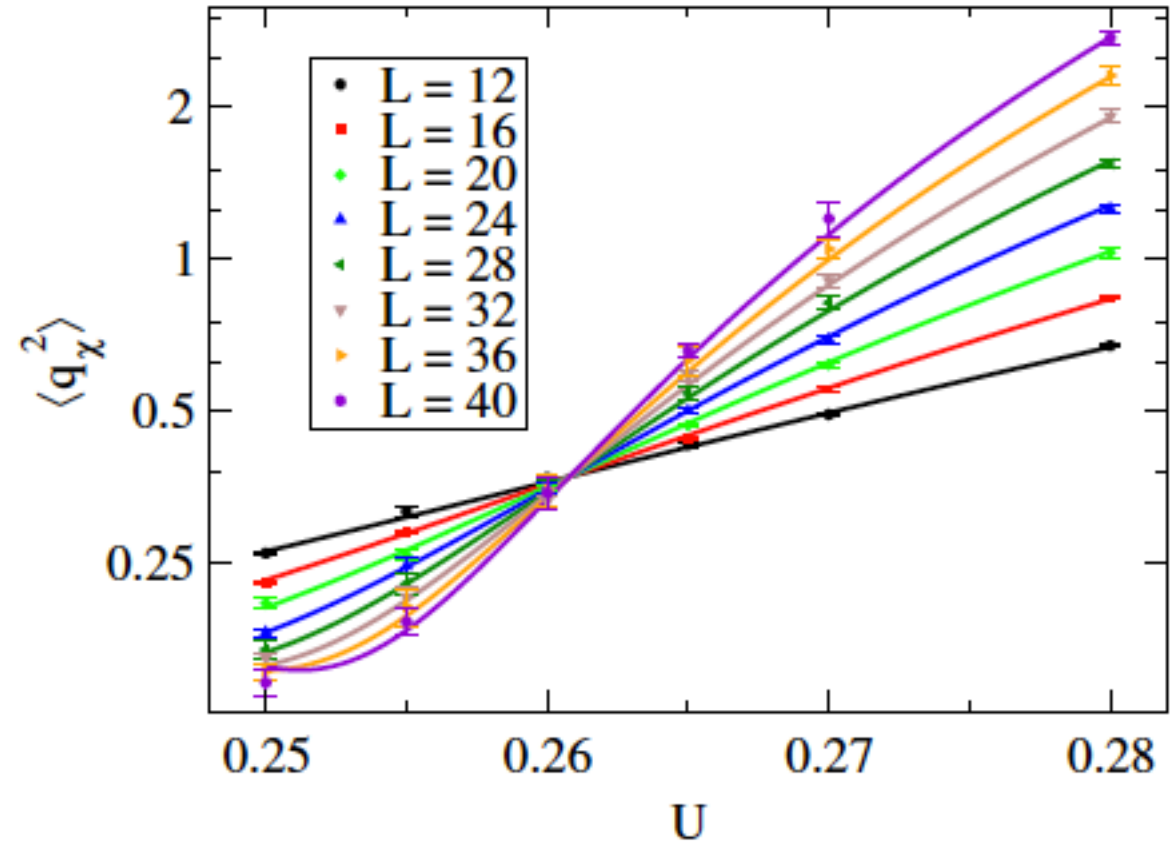

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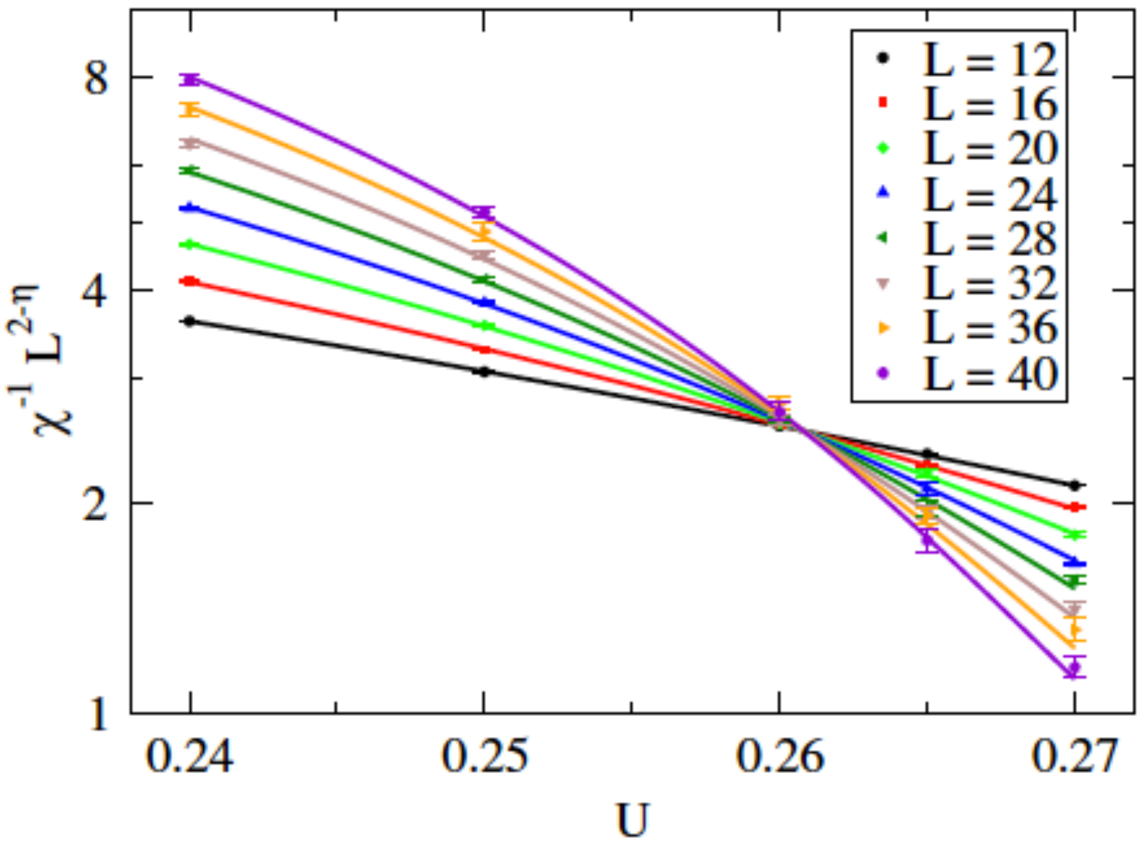

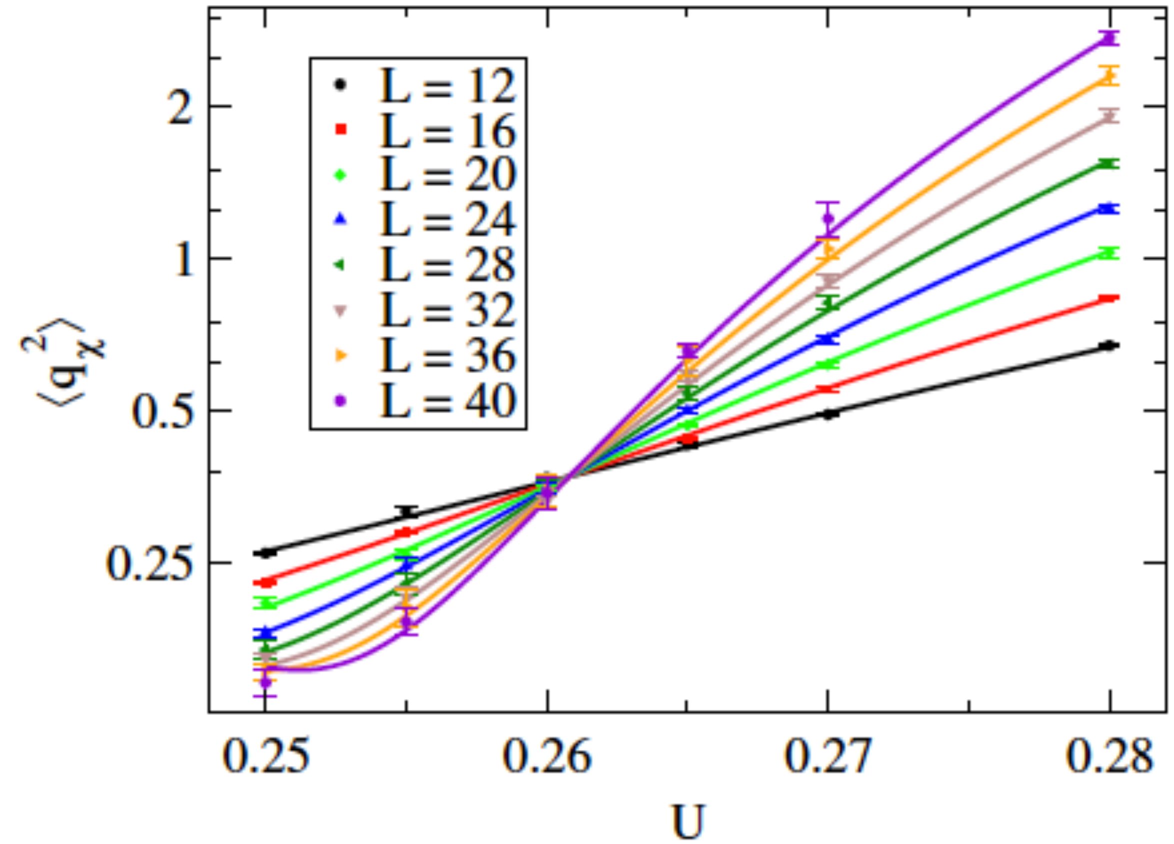

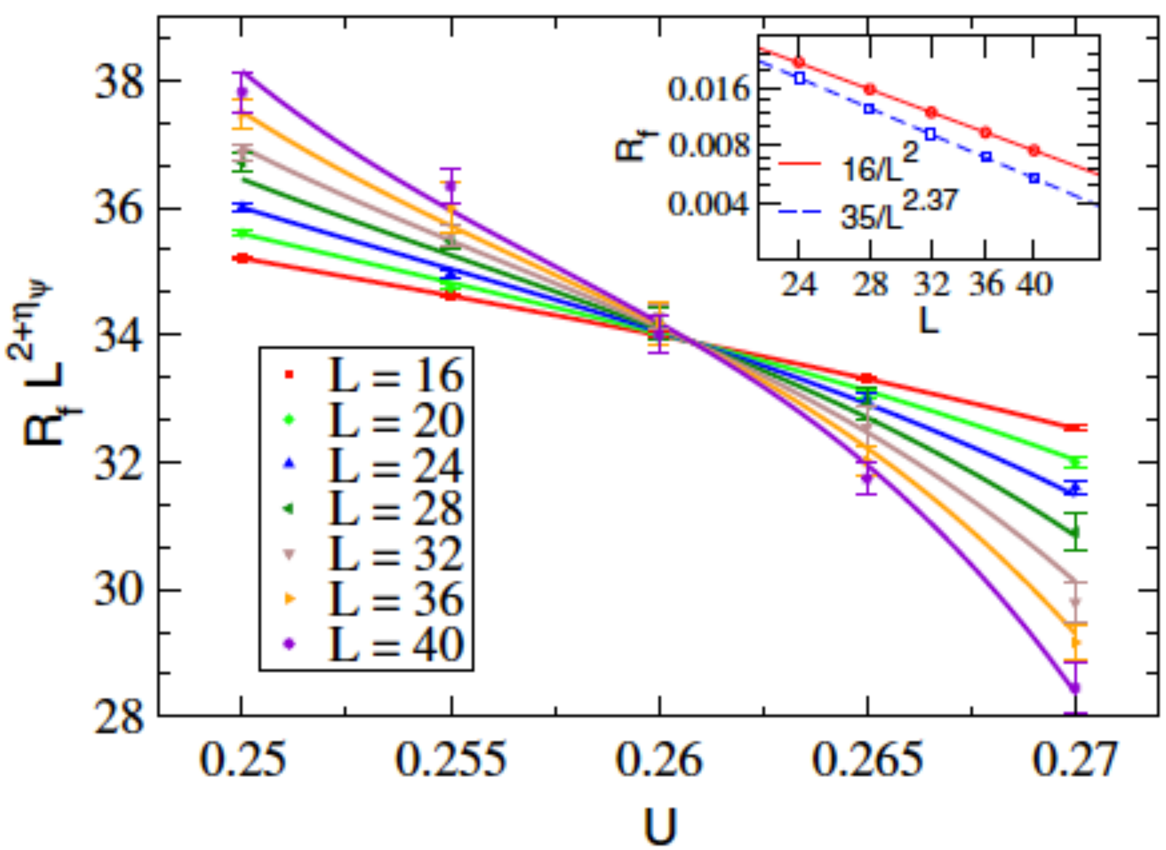

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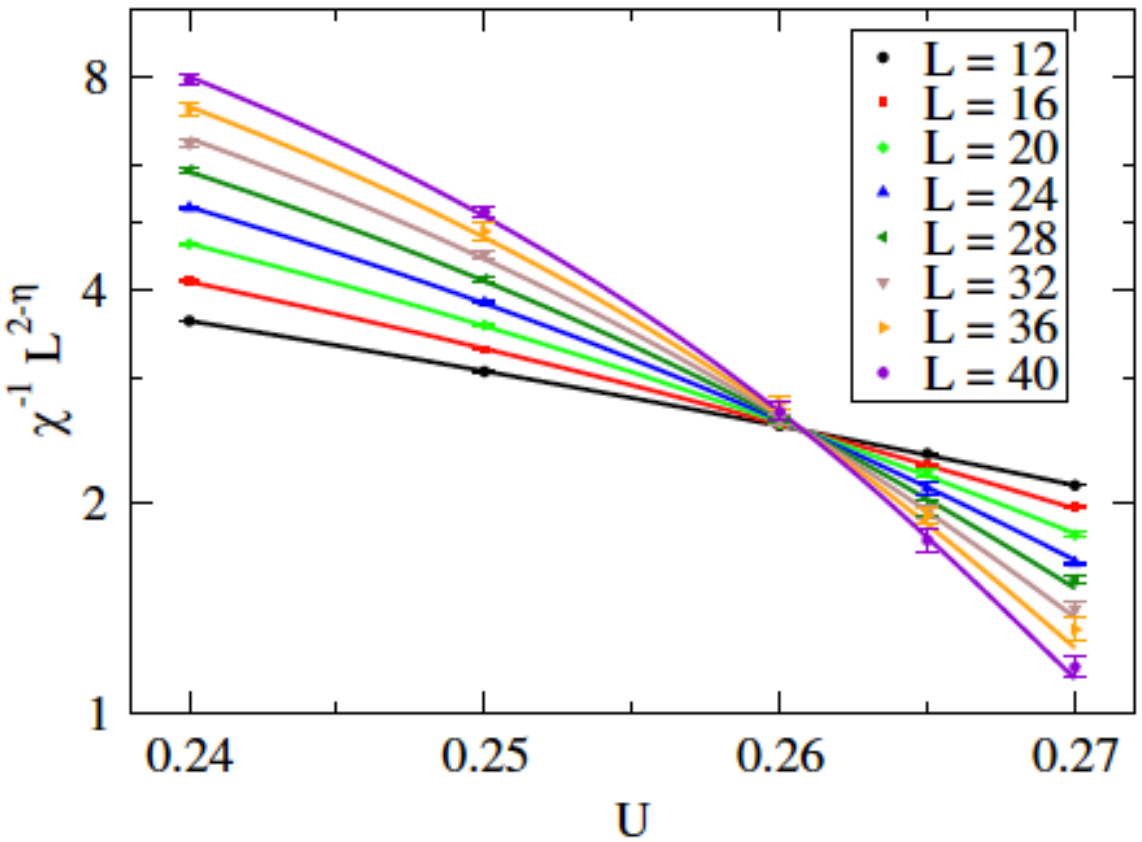

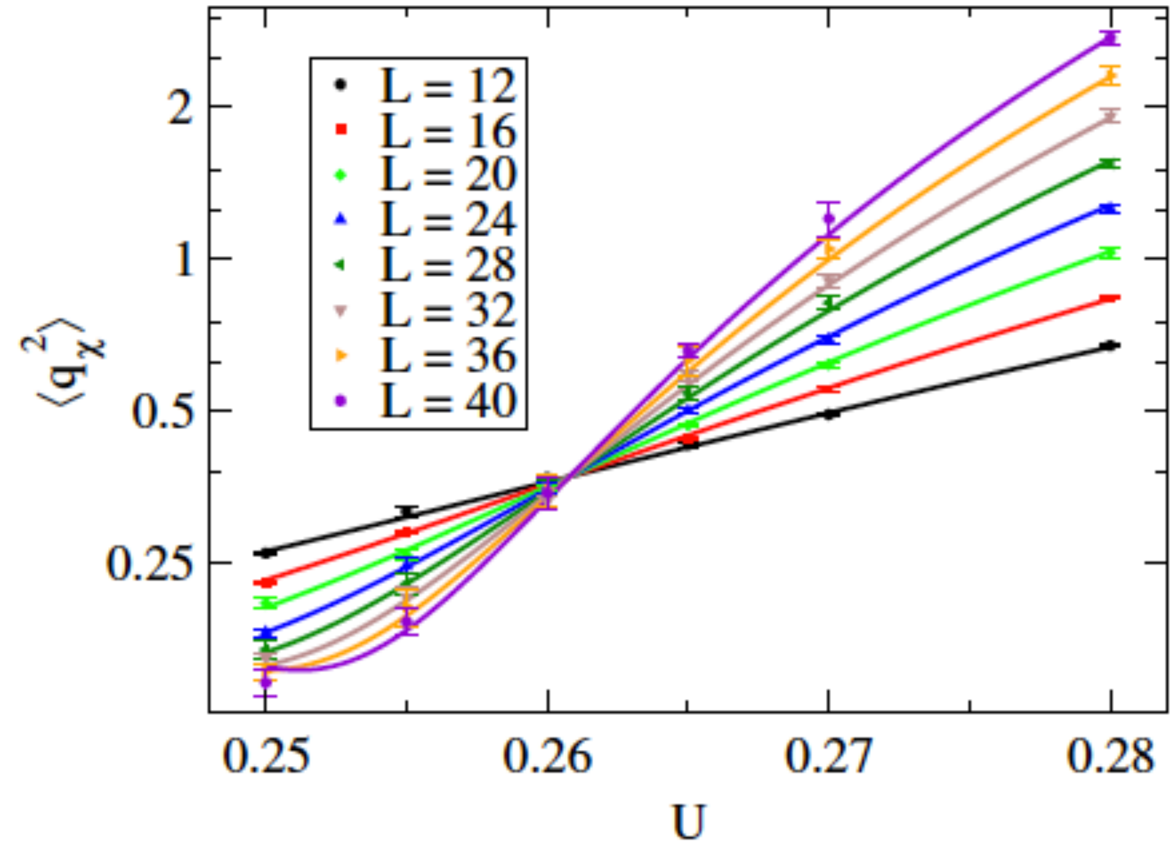

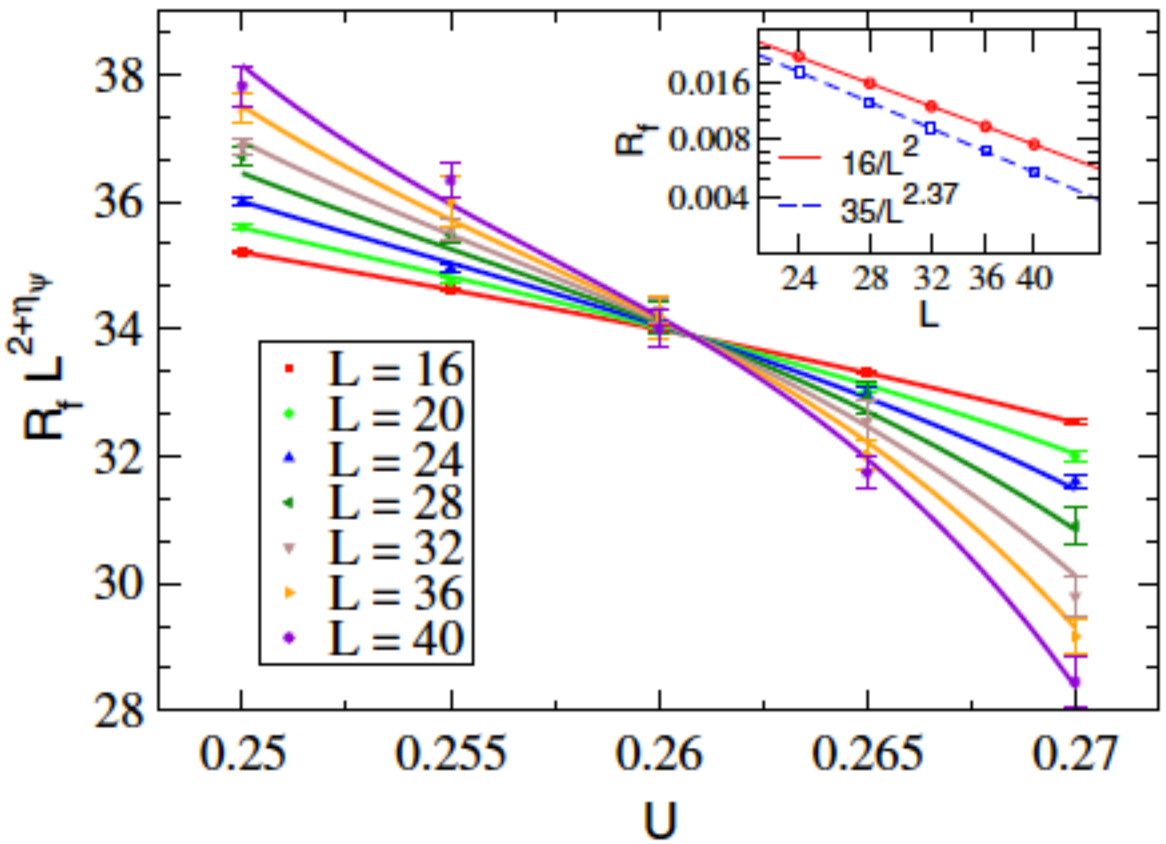

Combined fit results

$U_c = 0.2608(2)$

$\nu = 0.85(1)$

$\eta = 0.65(1)$

$\eta_\psi = 0.37(1)$

Previous work on Lattice Thirring Model

Previous work on Lattice Thirring Model

SU(2) x U(1) symmetric model

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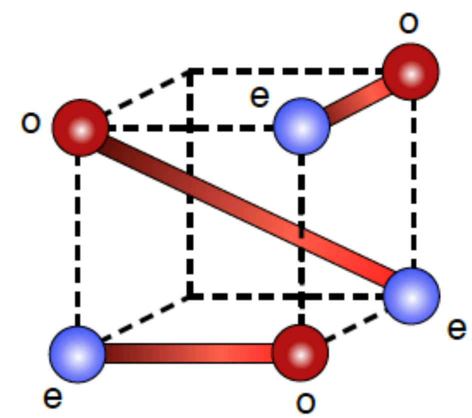
SU(2) x U(1) symmetric model

Work	Range of L	Range of m	U_c	ν	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) PRL, (2012)	12-40	0	0.2608(2)	0.85(1)	0.65(1)	0.37(1)

Gross-Neveu model results

Gross-Neveu model results



Gross-Neveu

Gross-Neveu model results

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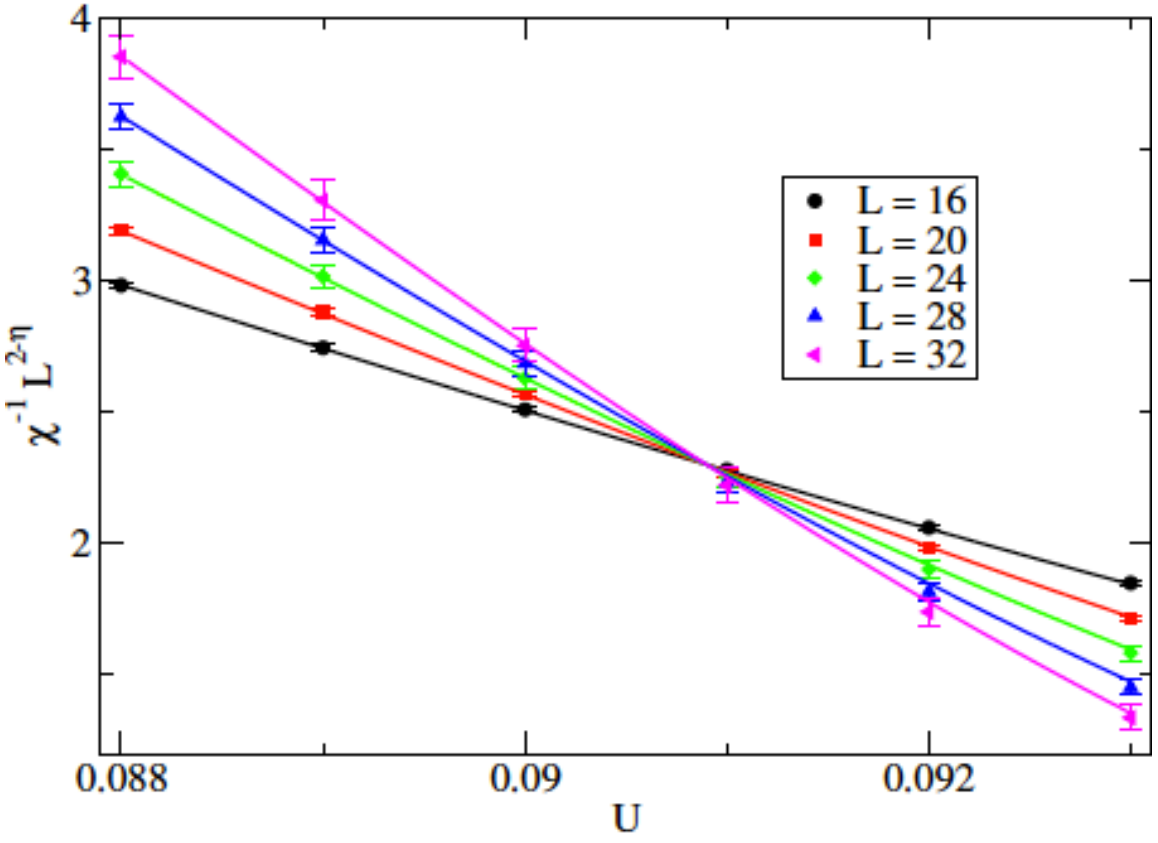

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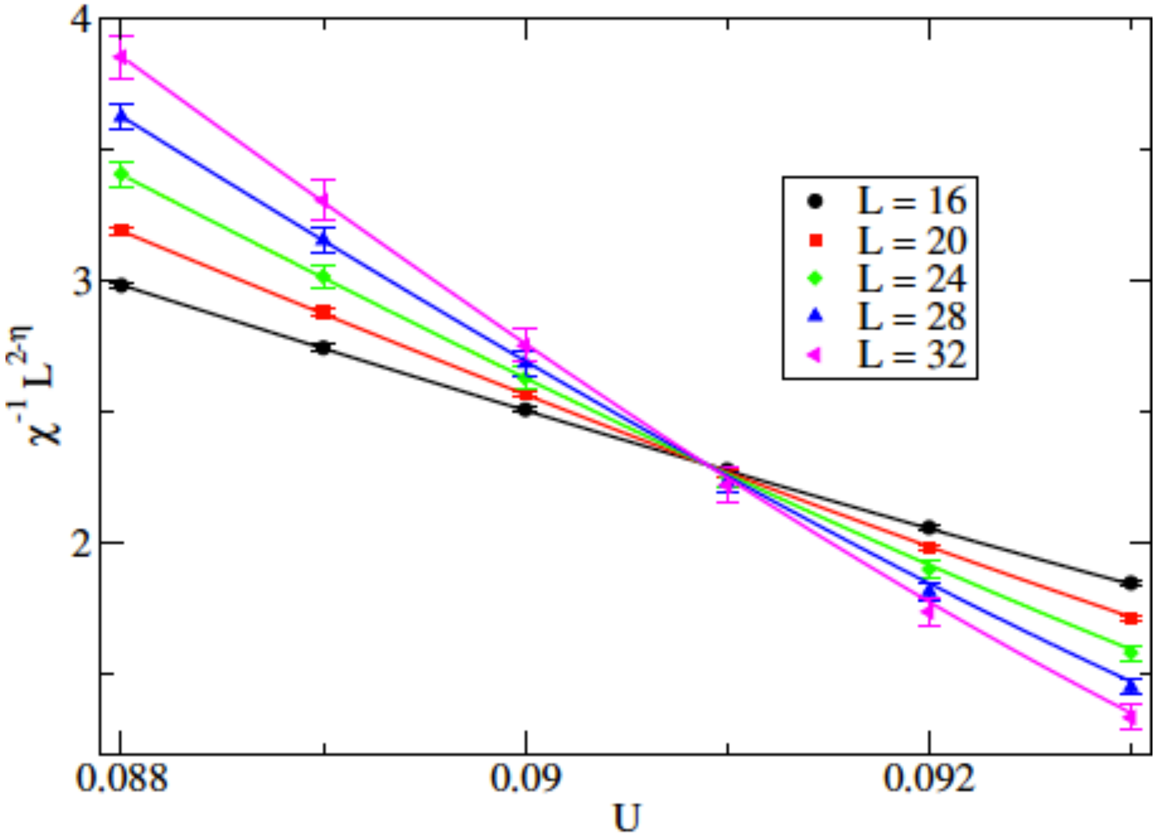

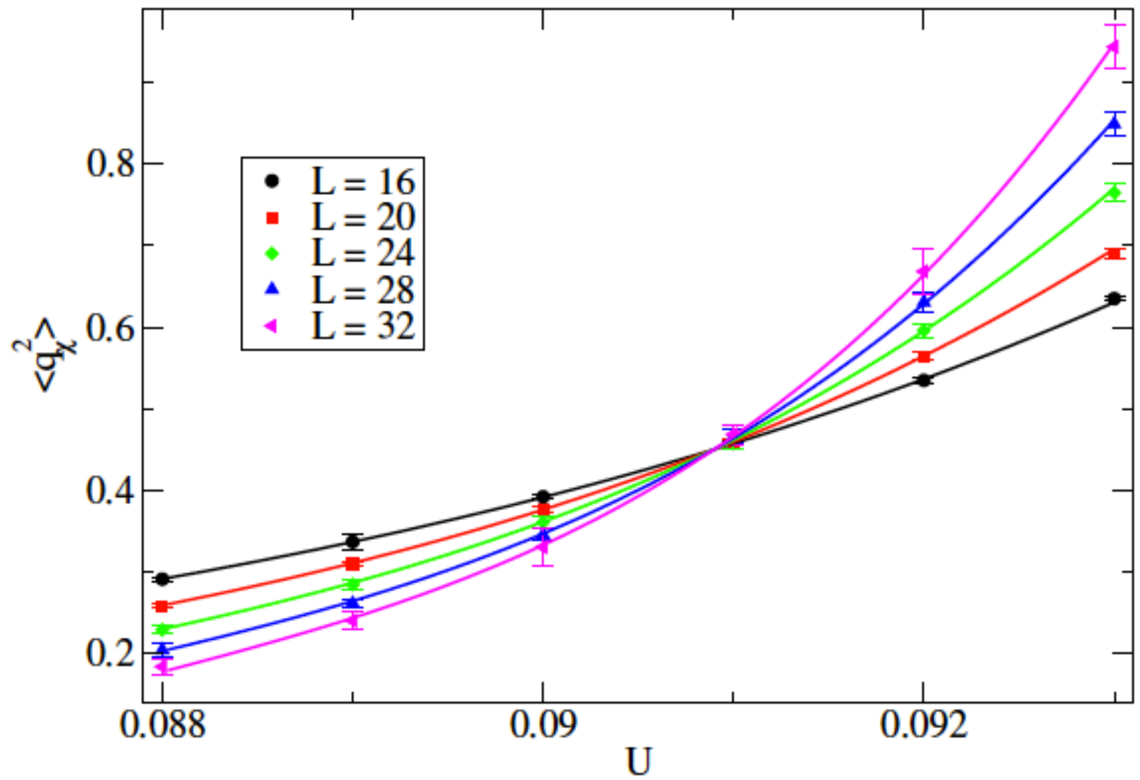

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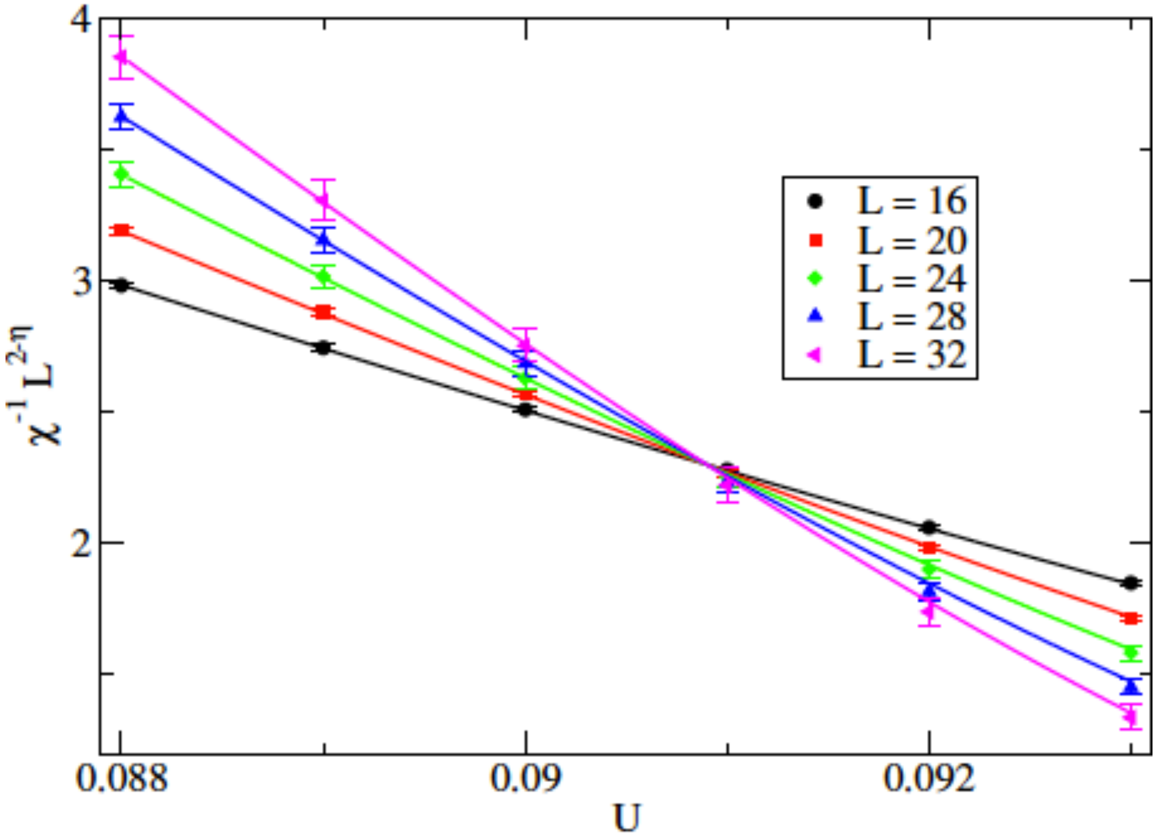

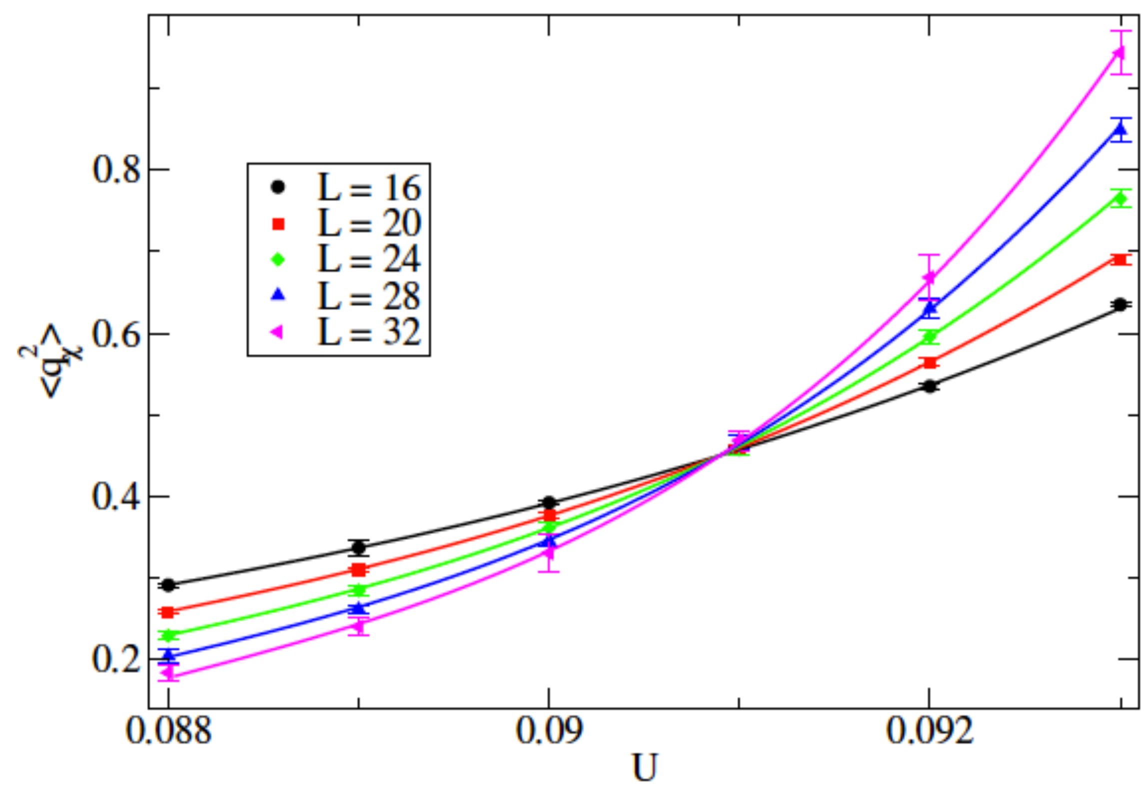

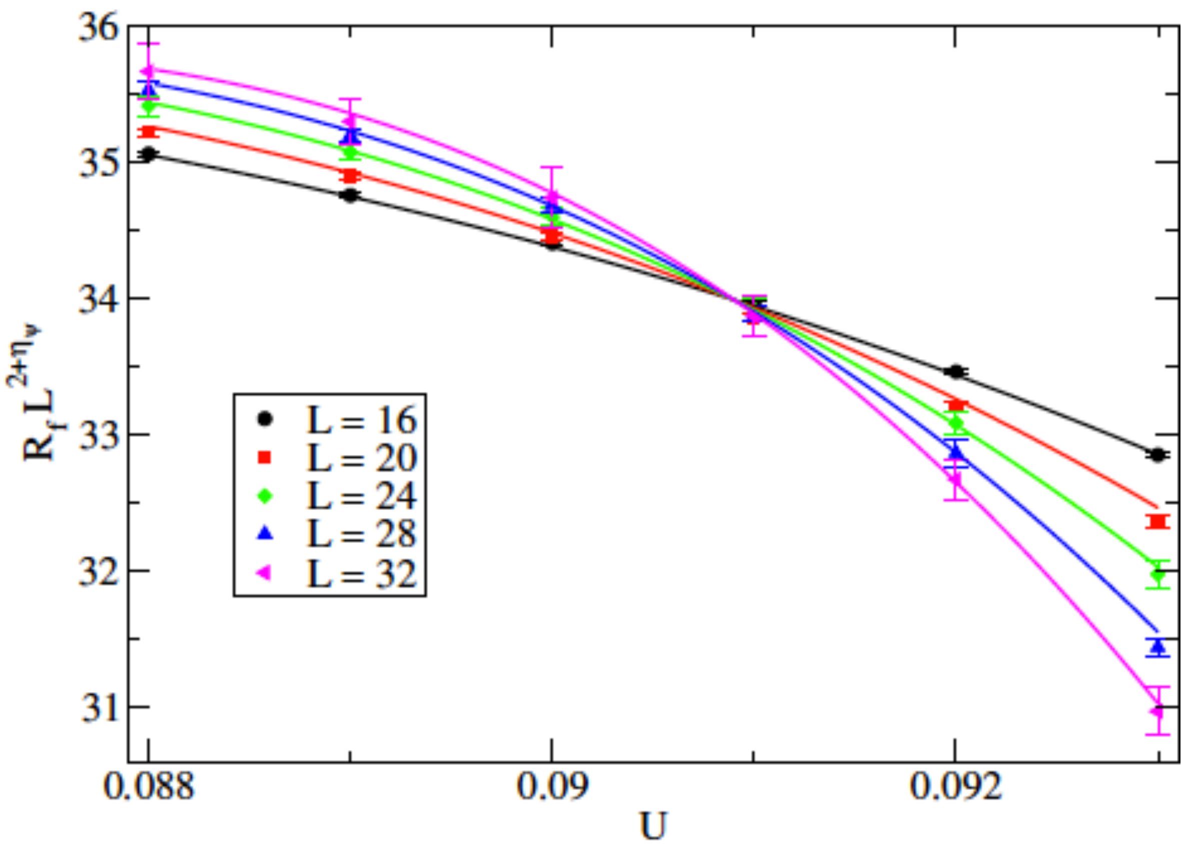

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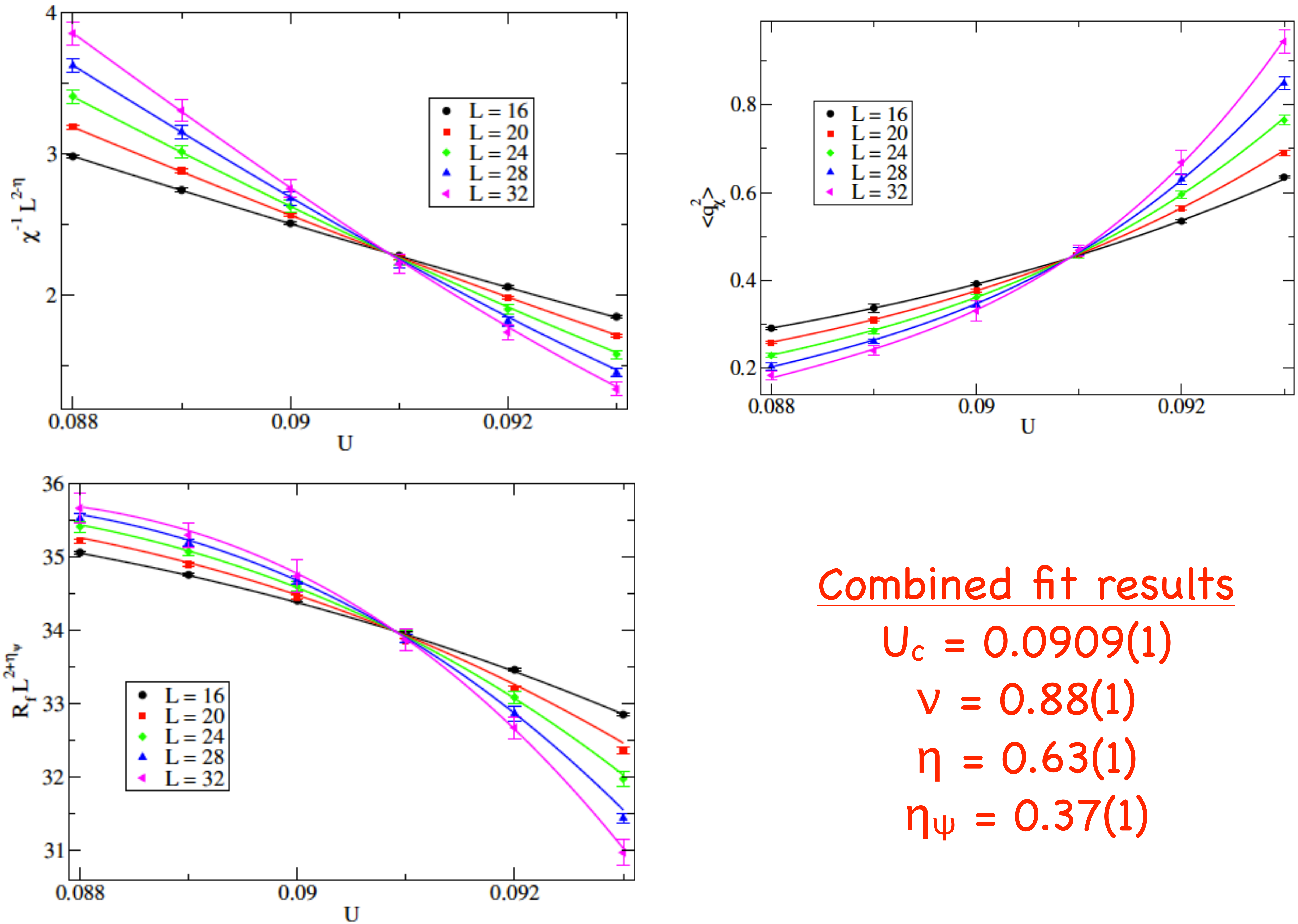

Combined fit results

$U_c = 0.0909(1)$

$\nu = 0.88(1)$

$\eta = 0.63(1)$

$\eta_\psi = 0.37(1)$

Previous work on Lattice GN Model

Previous work on Lattice GN Model

SU(Nf) x G symmetric model

Previous work on Lattice GN Model

SU(Nf) x G symmetric model

Work	Nf	G	ν	η
Christoffi & Strouthos JHEP05 (2007)088	4	Z2	0.99(2)	0.83(4)
		U(1)	1.03(4)	0.90(5)
		SU(2)	1.16(5)	1.10(6)
Karkkainen et. al., NPB415 (1994) 781	2	Z2	1.00(4)	0.754(8)
Rossa, Vitale and Wetterich PRL86 (2001) 958	2	Z2	1.0(5)	0.76(2)
Our Work	2	U(1)	0.88(1)	0.63(1)

Lattice Thirring versus GN models with same symmetries

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Do the phase transitions belong to the same universality class?

Lattice Thirring versus GN models with same symmetries

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Lattice Thirring versus GN models with same symmetries

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Traditional Belief : No!

GN models : Consistent with Large N

Thirring model : Not consistent with Large N

Lattice Thirring versus GN models with same symmetries

Do the phase transitions
belong to the same
universality class?

Traditional Belief : No!	Our finding : Yes!
GN models : Consistent with Large N	Clear deviations from Large N
Thirring model : Not consistent with Large N	We get the same critical exponents

Conclusions

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- Fermion bag approach is a new approach to strongly correlated fermion systems.

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- Calculations with exactly massless fermions feasible in “some” models.
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Future : Many new applications!