Diagrammatic Monte Carlo: Quantum Critical Points

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Special Lecture 2
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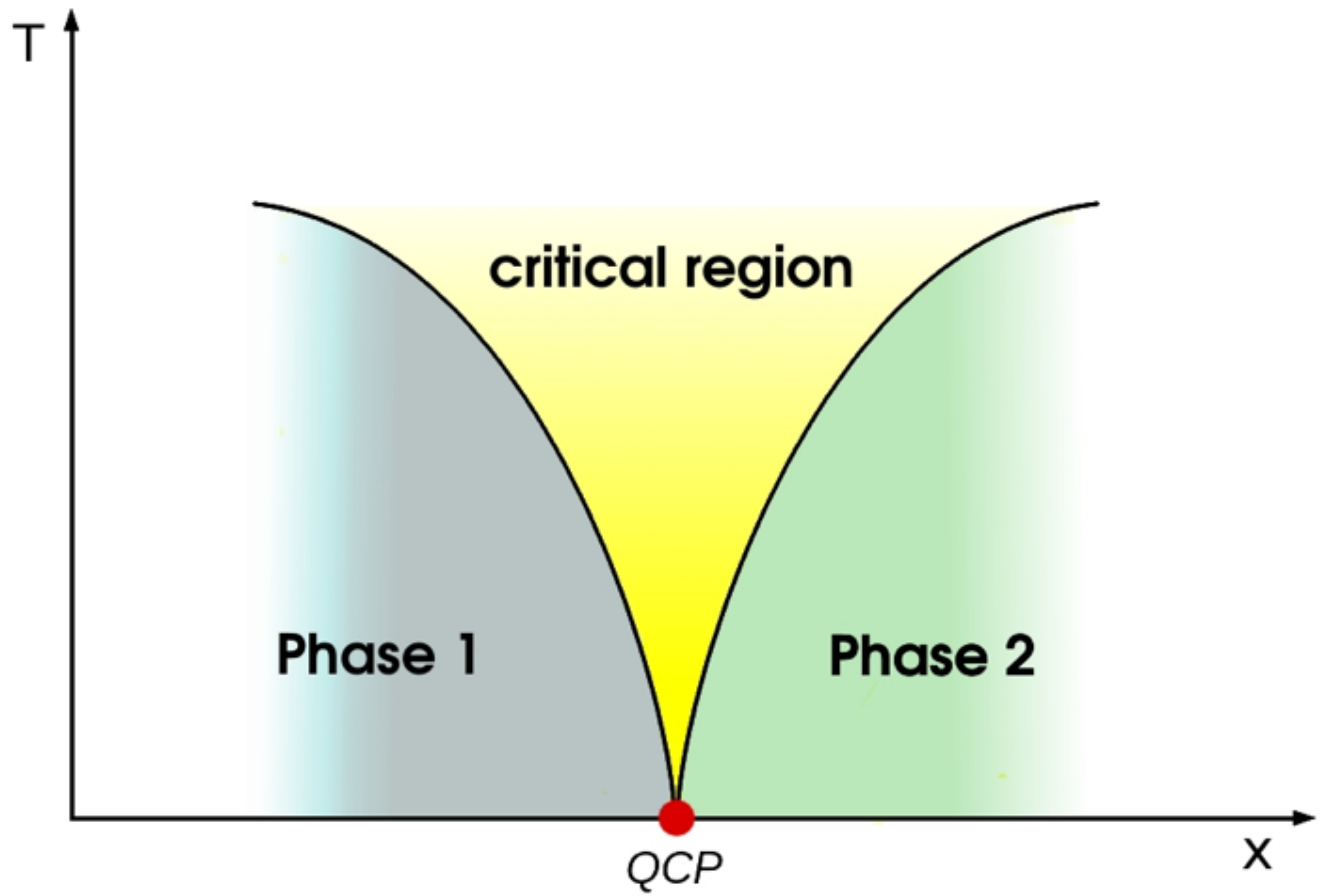
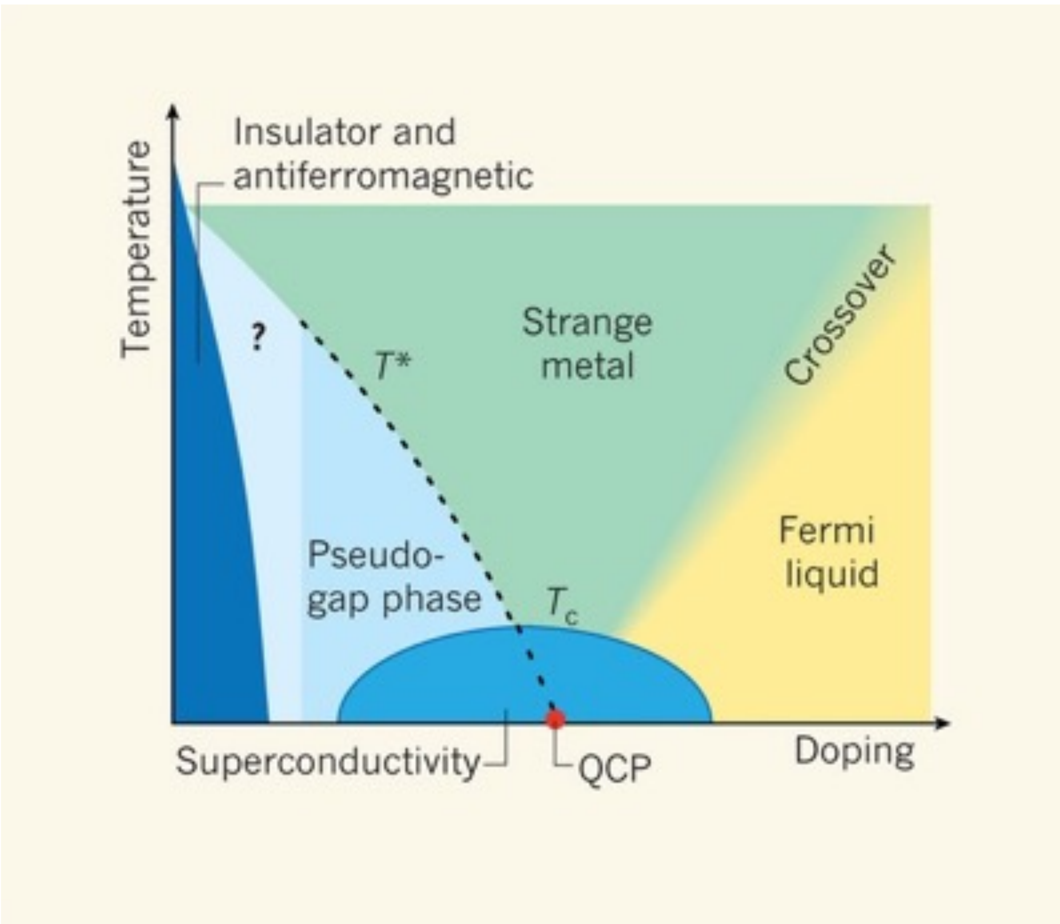
What is a Quantum Critical Point?

temperature

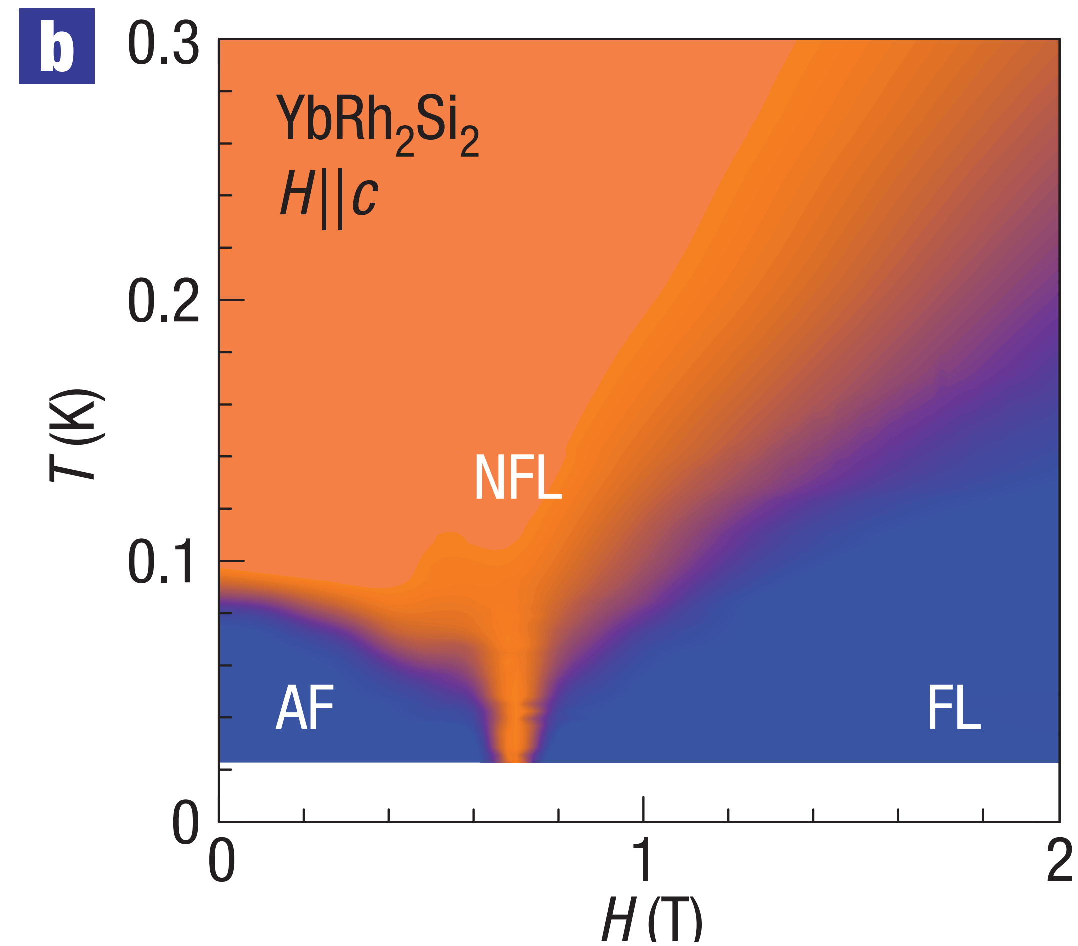


some tuning parameter

Many applications in CM



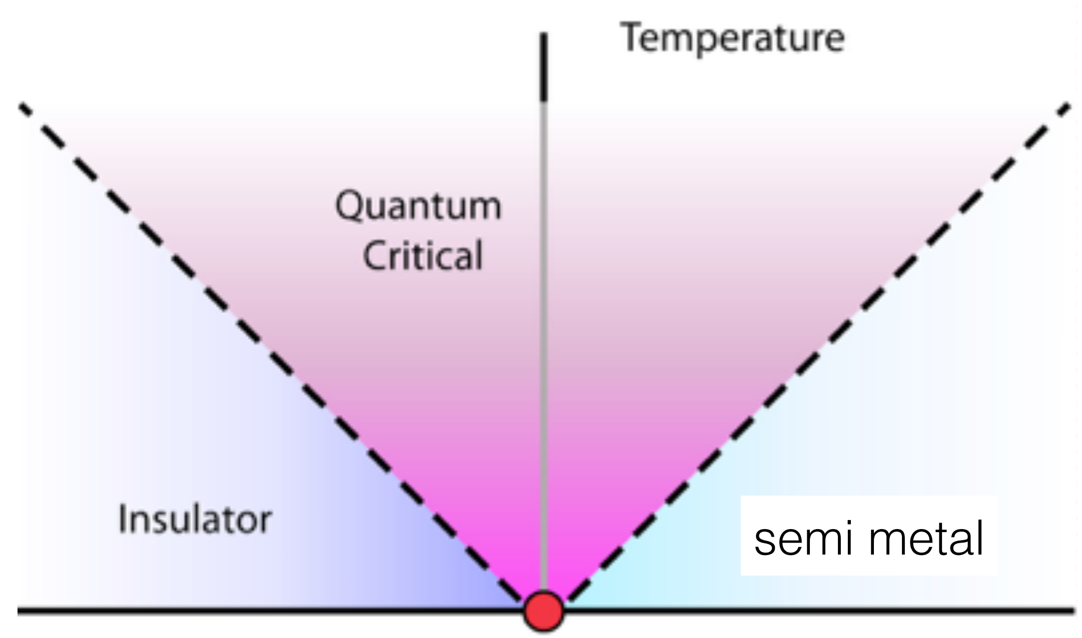
High Tc Materials



Heavy Fermion Systems

QCP's involving a fermi surface
usually suffer from severe sign problems

Semimetal - Insulator transitions are sometimes free of sign problems.



Can be studied using
lattice models with four-fermion couplings

Hands, Del Debbio, Strouthos,
Drut, Lahde,
...

Diagrammatic methods offer a
new approach to study these problems

We will consider two applications in this talk!

The 3D Lattice Thirring Model

SC (2010), SC & A. Li (2012)

Action

$$S = \sum_{x,\alpha} \left\{ \frac{1}{2}\eta_{x,\alpha}\left(\overline{\psi}_x\psi_{x+\alpha} - \overline{\psi}_{x+\alpha}\psi_x\right) + U\ \overline{\psi}_x\psi_{x+\alpha}\overline{\psi}_{x+\alpha}\psi_x \right\}$$

free massless staggered fermions

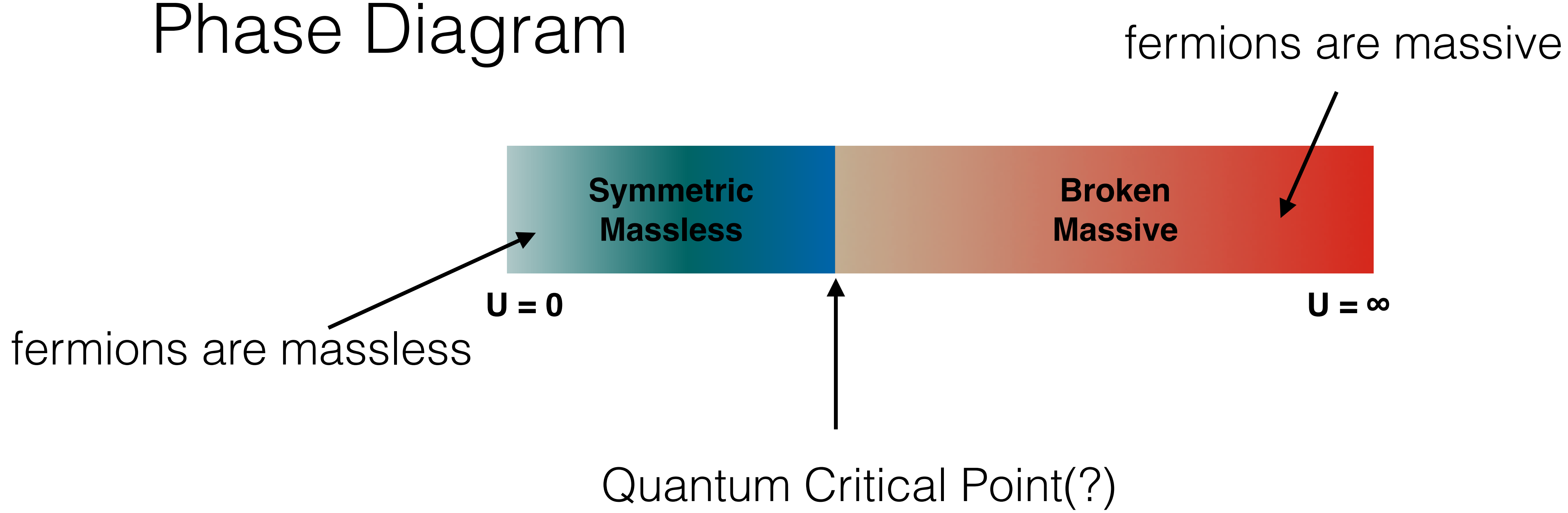
nearest neighbor four-fermion coupling

U(1) chiral symmetry: $\psi_x \to e^{i\varepsilon_x\theta}\psi_x, \quad \overline{\psi}_x \to \overline{\psi}_x e^{i\varepsilon_x\theta}$

analogous to the axial symmetry of Dirac fermions in 4d

$$\psi_x \to e^{i\gamma_5\theta}\psi_x, \quad \overline{\psi}_x \to \overline{\psi}_x e^{i\gamma_5\theta}$$

Phase Diagram



Order parameter: chiral condensate

$$\langle \overline{\psi}\psi \rangle = \frac{1}{Z} \int [d\overline{\psi} d\psi] \, e^{-S} \, \overline{\psi}_x \psi_x$$

Symmetric
Massless Phase

$$\langle \overline{\psi}\psi \rangle = 0$$

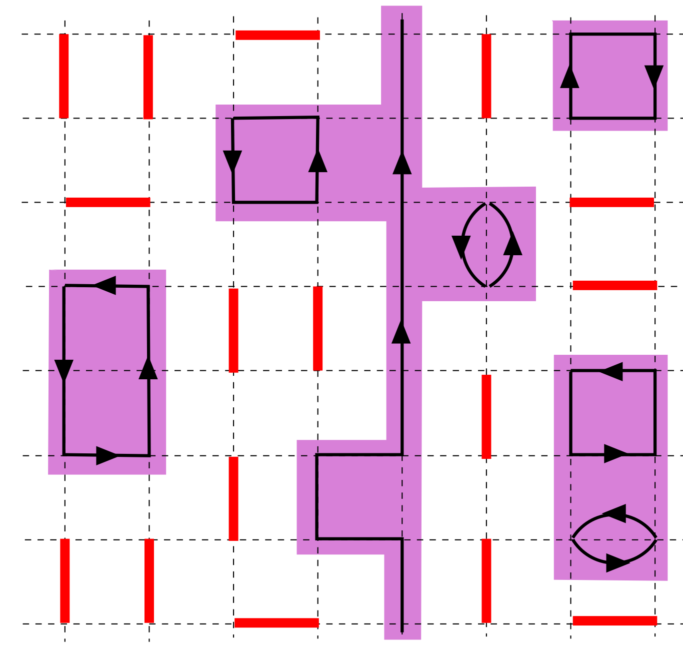
Broken
Massive Phase

$$\langle \overline{\psi}\psi \rangle \neq 0$$

Partition function

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

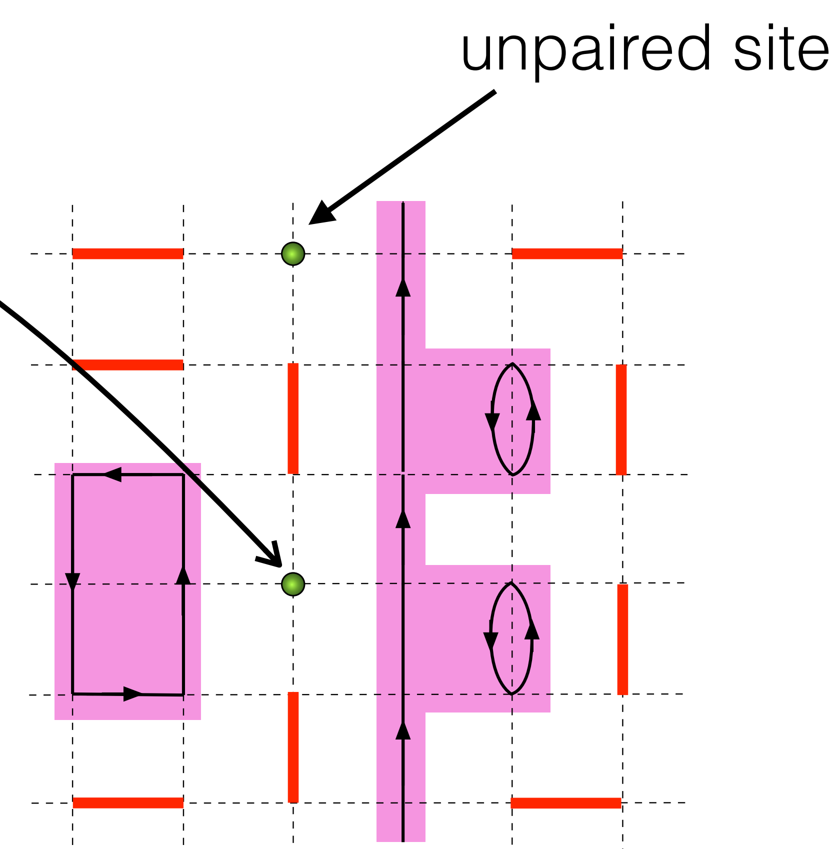
$$W_{\text{Bag}} = \begin{array}{c c c c} & \text{even} & \text{odd} & \\ & \left(\begin{array}{c} 0 \\ -A^T_{\text{Bag}} \end{array} \right. & \left. \begin{array}{c} A_{\text{Bag}} \\ 0 \end{array} \right) & \begin{array}{c} \text{even} \\ \text{odd} \end{array} \end{array}$$



chiral condensate

$$\langle \overline{\psi}\psi \rangle = \frac{1}{Z} \int [d\overline{\psi} d\psi]\, e^{-S}\, \overline{\psi}_x \psi_x$$

$= 0$ in a finite volume due to symmetry!



There will be another unpaired site somewhere!

$$\langle \overline{\psi}_x \psi_x\, \overline{\psi}_y \psi_y \rangle = \int [d\overline{\psi} d\psi]\, e^{-S}\, \overline{\psi}_x \psi_x\, \overline{\psi}_y \psi_y$$

can be non-zero!

Chiral Susceptibility

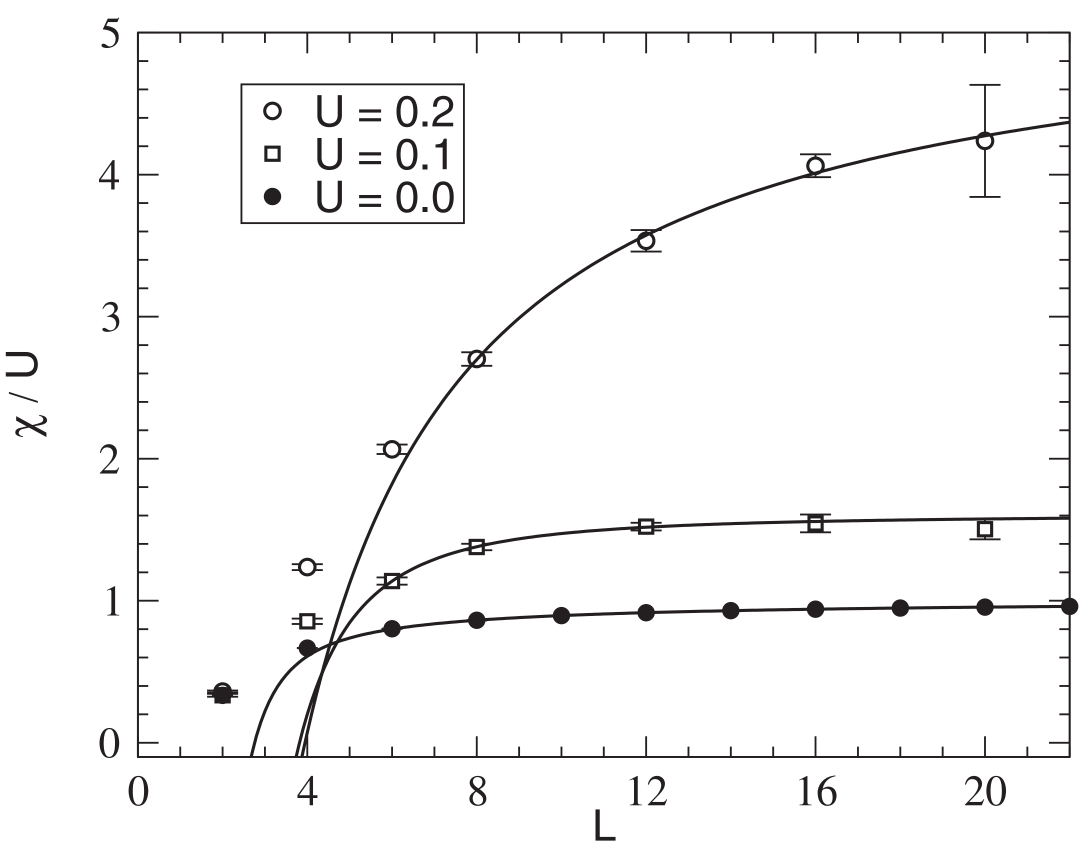
$$\chi = \frac{1}{V} \sum_{x,y} \langle \overline{\psi}_x \psi_x \; \overline{\psi}_y \psi_y \rangle$$

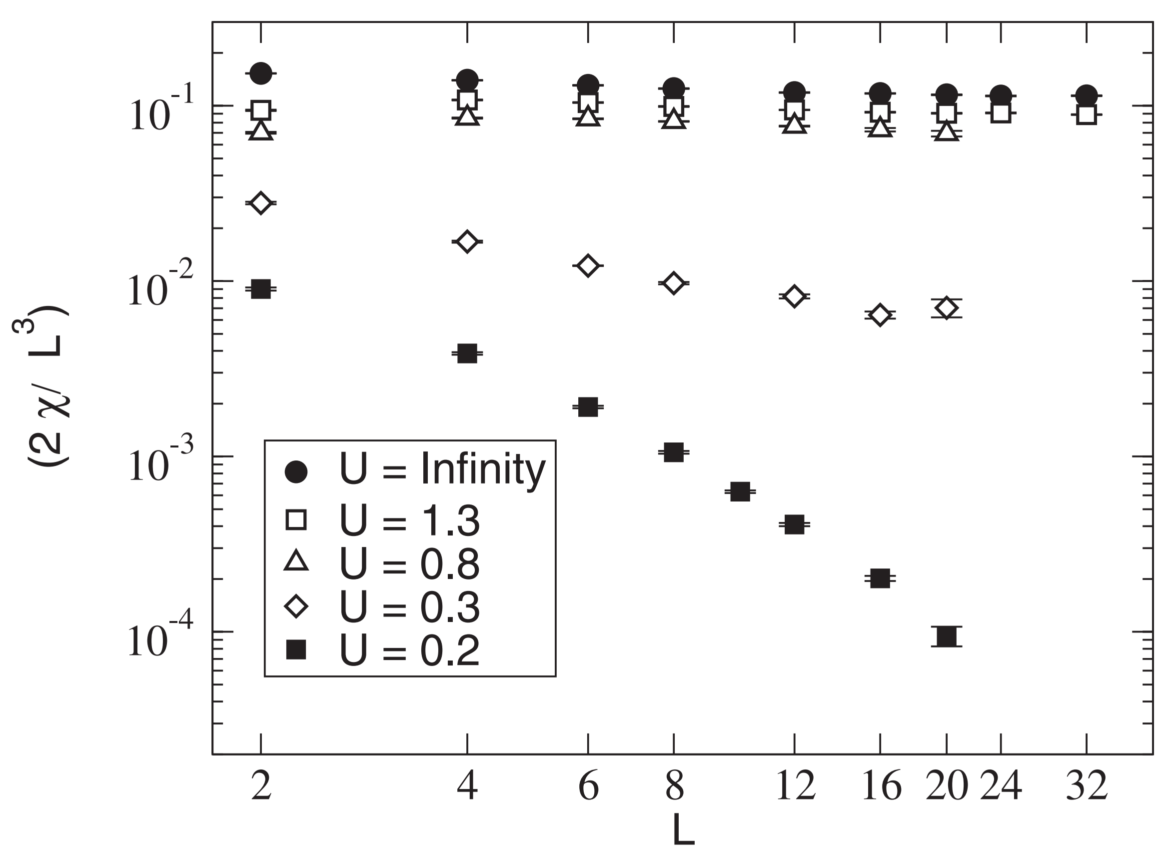
symmetric
massless phase

$\chi \sim$ Const.

broken
massive phase

$\chi \sim V$

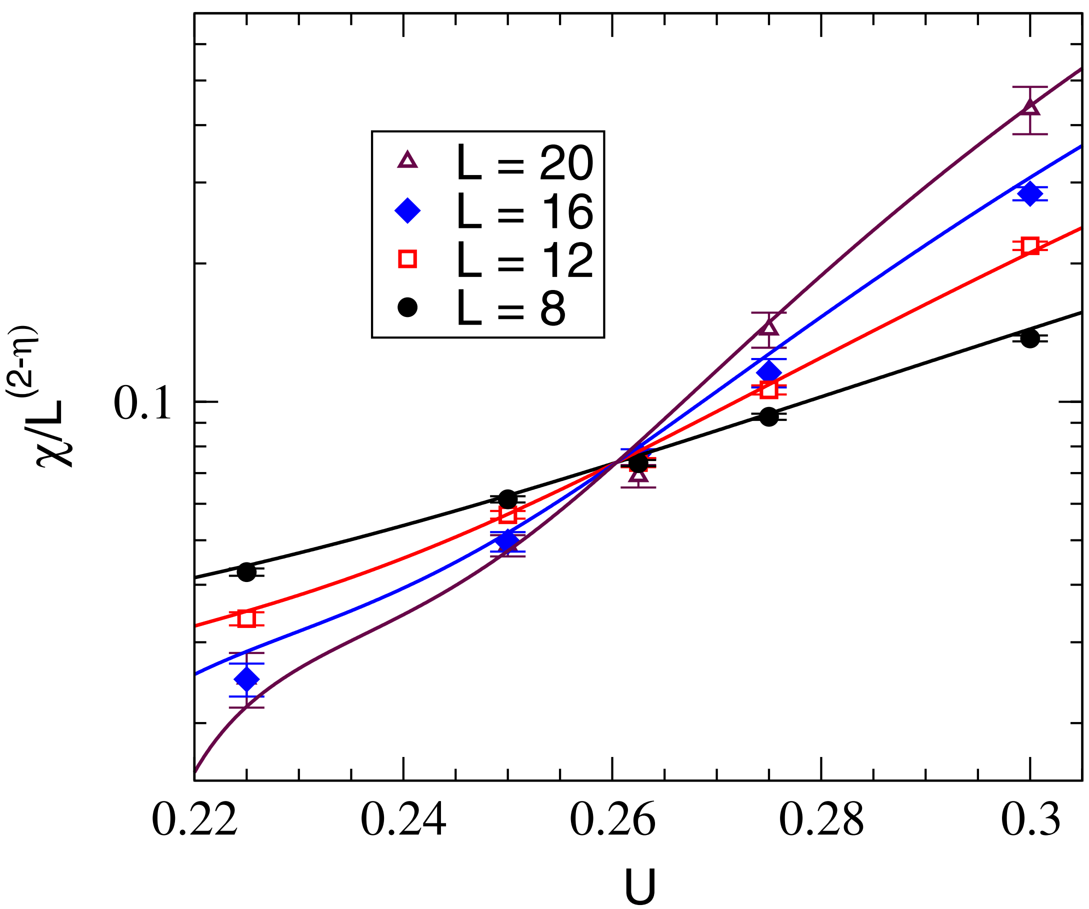




Critical Point

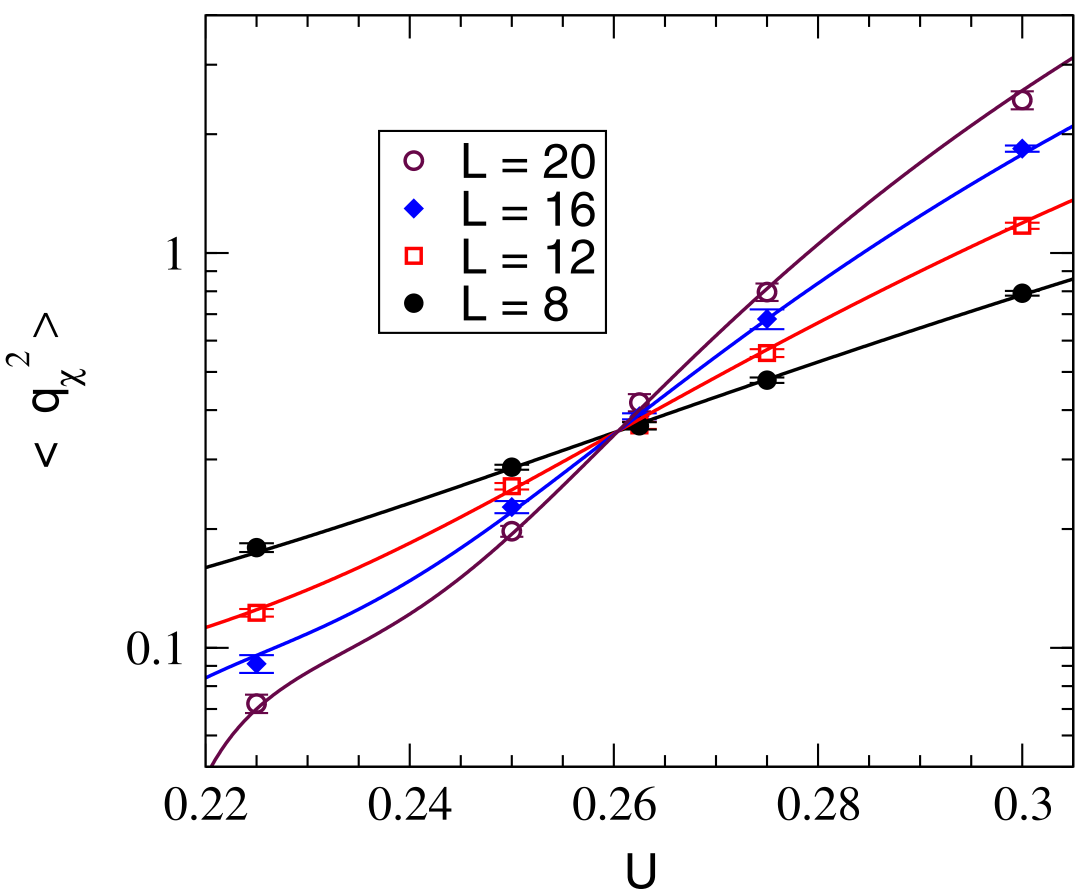
chiral condensate susceptibility

$$\chi \sim L^{2-\eta}$$



chiral charge susceptibility

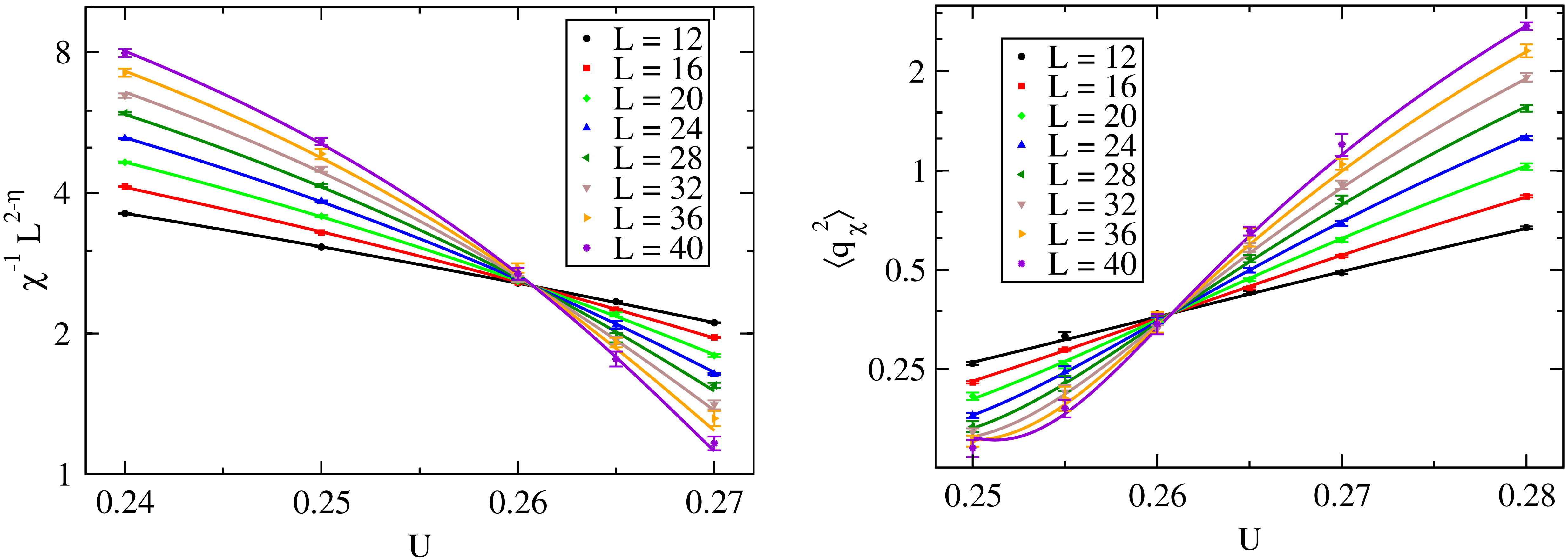
$$\langle q_\chi^2 \rangle \sim \text{Const.}$$



It is easy to locate the critical point!

Larger Lattice Results

SC, A.Li, PRL108 (2012) 140404



<u>Combined fit results</u>

$U_c = 0.2608(2)$

$\nu = 0.85(1)$

$\eta = 0.65(1)$

Traditional vs. Diagrammatic

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	1	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)

A 3D Lattice Gross-Neveu Model

Action

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

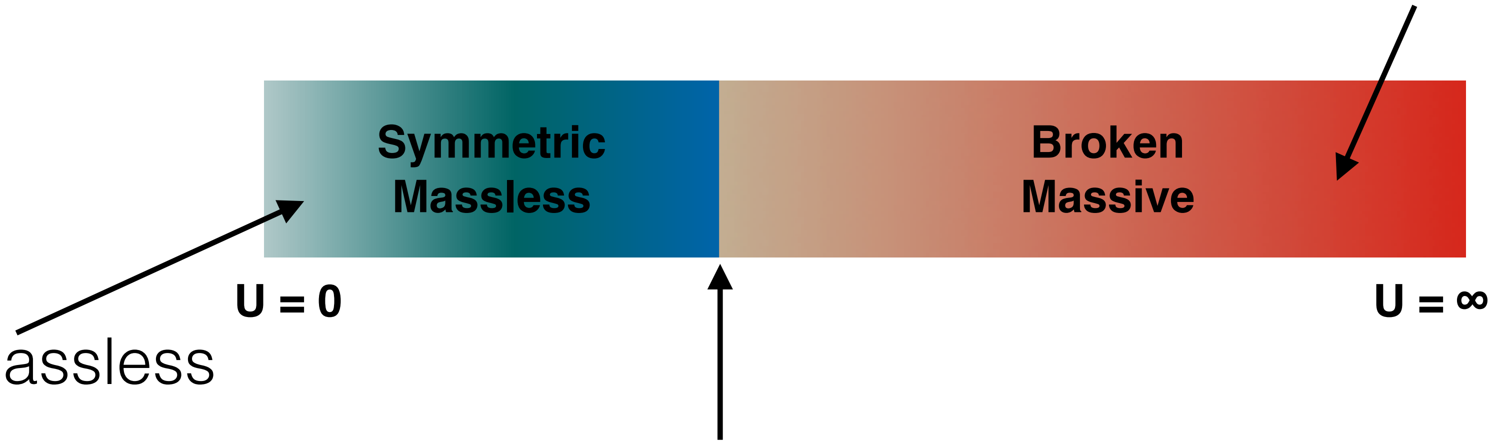
N_f = 4 reduced massless staggered fermions

onsite four-fermion coupling

SU(4) chiral symmetry:

$$\psi_{x,a} \to \sum_{b} V_{ab}\ \psi_{x,b}, \ \text{even sites}, \quad \psi_{x,a} \to \sum_{b} V^{*}_{ab}\ \psi_{x,b}, \ \text{odd sites}$$

Phase Diagram: Conventional Wisdom



Order parameter

$$\langle \psi_a \psi_b \rangle \; = \; \frac{1}{Z} \int [d\psi] \, e^{-S} \; \psi_{x,a} \psi_{x,b}$$

Symmetric
Massless Phase

$$\langle \psi_a \psi_b \rangle \; = \; 0$$

Broken
Massive Phase

$$\langle \psi_a \psi_b \rangle \; \neq \; 0$$

There is more to the story!

Diagrammatic Approach

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

$$Z = \int [d\psi]\ \mathrm{e}^{-\frac{1}{2}\psi^T M \psi} \prod_{x} \left(1\ +\ U\ \psi_{x,1}\psi_{x,2}\psi_{x,3}\psi_{x,4}\right)$$

$$Z = \sum_{[n]} U^k \int [d\psi]\ \mathrm{e}^{-\frac{1}{2}\psi^T M \psi}\ \psi_{x_1,1}\psi_{x_1,2}\psi_{x_1,3}\psi_{x_1,4}\ \ldots\ \psi_{x_k,1}\psi_{x_k,2}\psi_{x_k,3}\psi_{x_k,4}$$

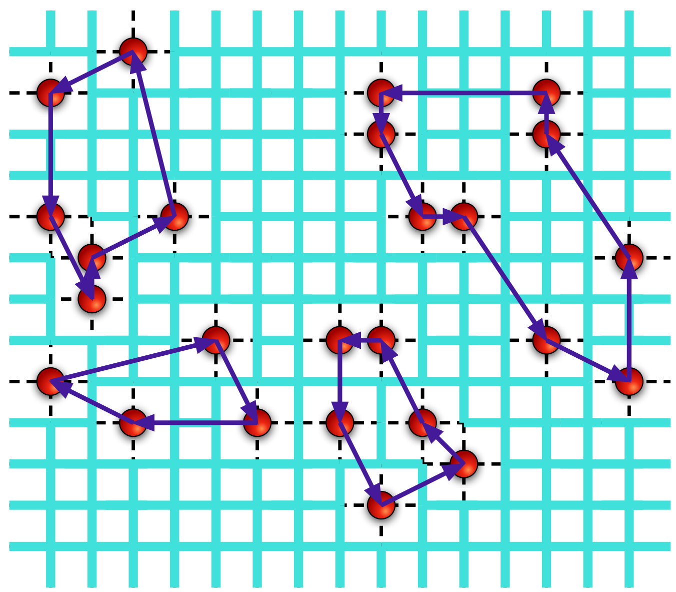
monomer field

$$Z = \sum_{[n]} U^k \int [d\psi]\ e^{-\frac{1}{2}\psi^T M \psi}\ \psi_{x_1,1}\psi_{x_1,2}\psi_{x_1,3}\psi_{x_1,4}\ \ldots\ \psi_{x_k,1}\psi_{x_k,2}\psi_{x_k,3}\psi_{x_k,4}$$

Weak coupling approach:

$$Z = \Big(\mathrm{Pf}(M)\Big)^4 \sum_{[n]} U^k \Big(\mathrm{Pf}(G)\Big)^4$$

G is a k x k matrix



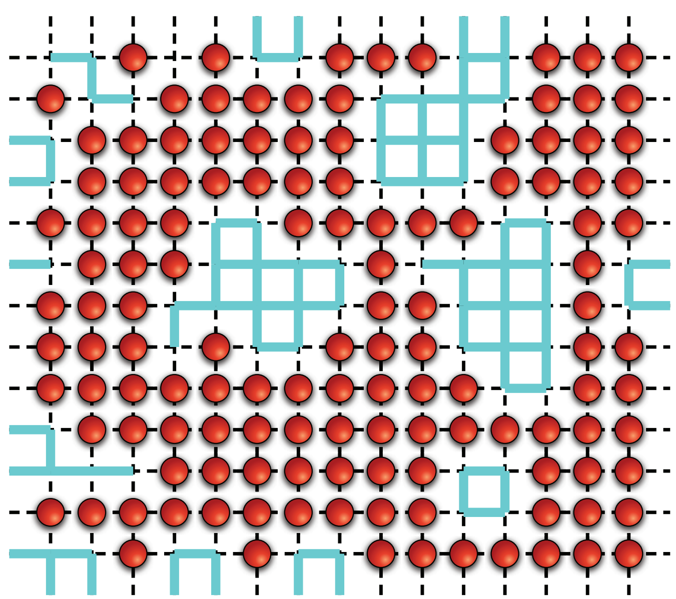
Weak Coupling Diagrams

Duality

Strong coupling approach:

$$Z = \sum_{[n]} U^k \prod_{\mathrm{Bags}} \Big(\mathrm{Pf}(W_{\mathrm{Bag}})\Big)^4$$

W is a (V-k) x (V-k) matrix



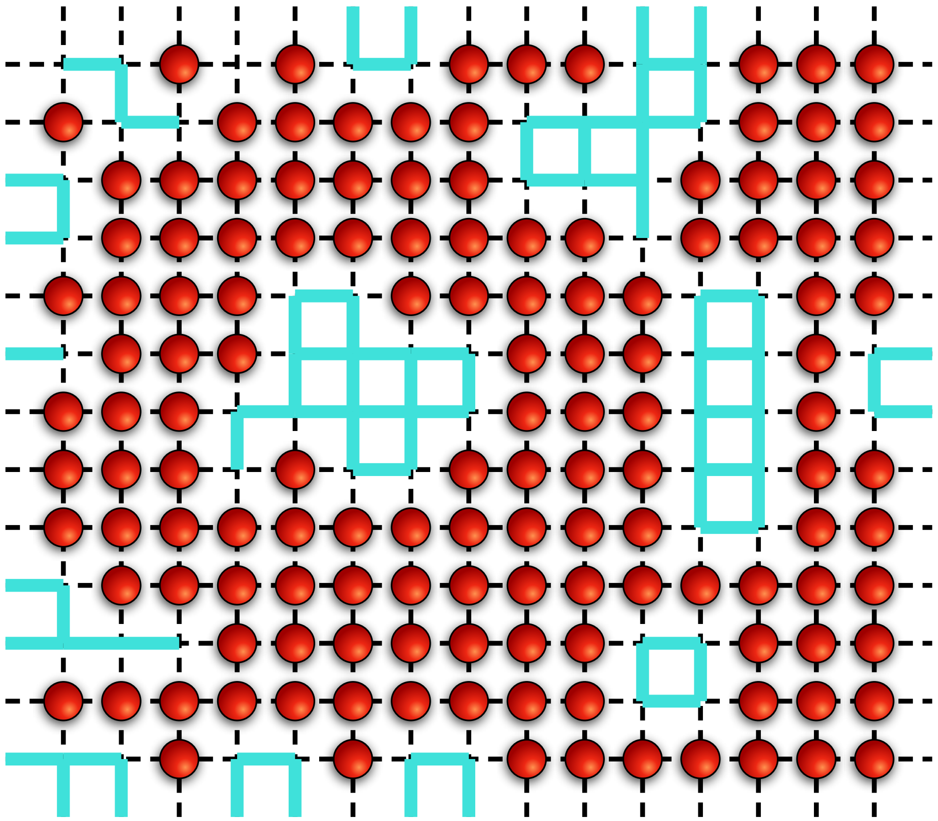
Strong Coupling Diagrams

A useful Property of W_{Bag}

$$Z = \sum_{[n]} U^k \prod_{\text{Bags}} \left(\text{Pf}(W_{\text{Bag}})\right)^4$$

$$\begin{array}{ccc} & \text{even} & \text{odd} & \\ W_{\text{Bag}} = & \left(\begin{array}{cc} 0 & A_{\text{Bag}} \\ -A^T_{\text{Bag}} & 0 \end{array} \right) & & \begin{array}{c} \text{even} \\ \text{odd} \end{array} \end{array}$$

$$Pf(W_{\text{Bag}}) = \text{Det}(A_{\text{Bag}})$$



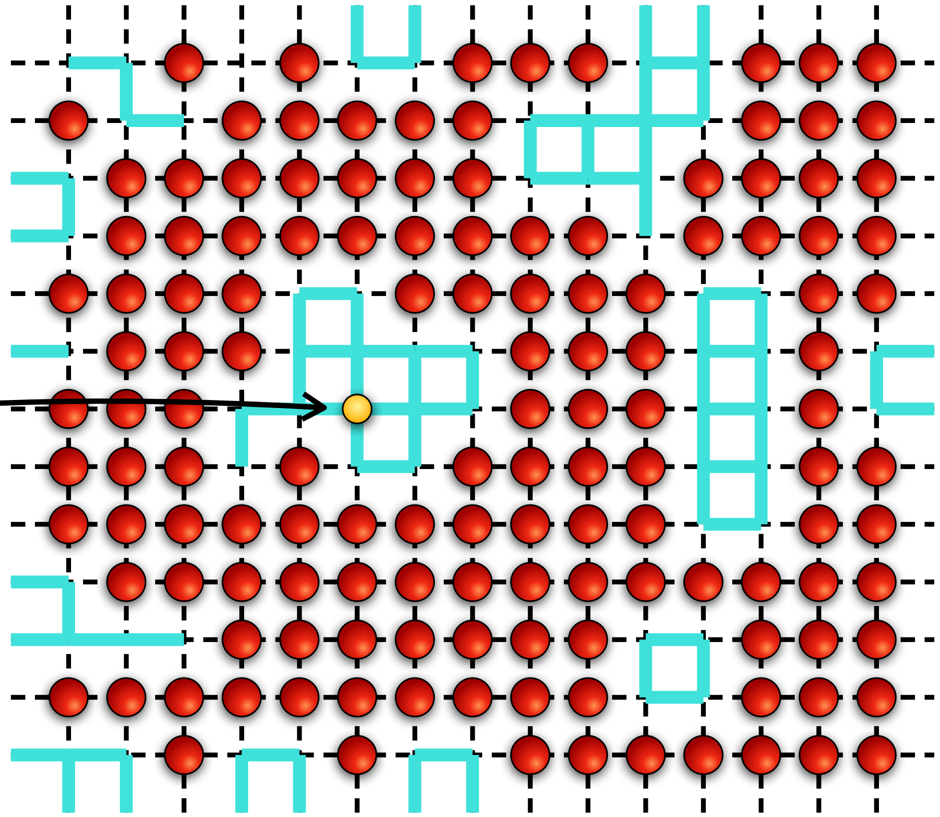
If a bag has unequal number of even and odd sites its weight vanishes!

chiral condensate

$$\langle \psi_a \psi_b \rangle = \frac{1}{Z} \int [d\psi]\, \mathrm{e}^{-S}\, \psi_{x,a} \psi_{x,b}$$

$$\langle\ \psi_a\ \psi_b\ \rangle = 0$$

in a finite volume
due to symmetry



fermion bag containing the condensate
has zero weight

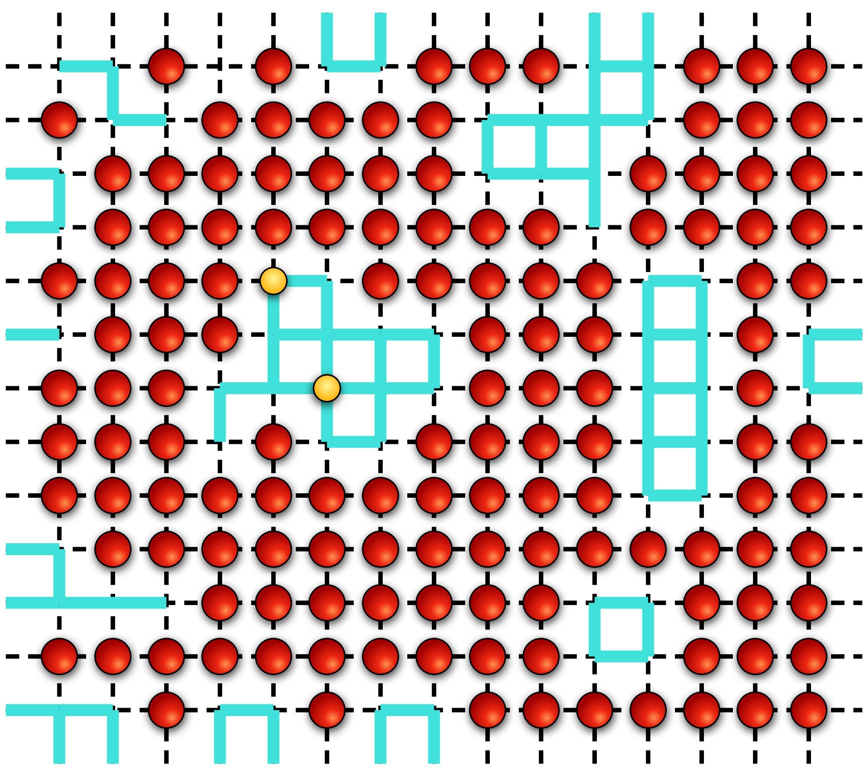
for two flavors the site has to be dropped while
computing the weight of the fermion bag containing the site

for two other flavors the site has to be kept while
computing the weight of the fermion bag containing the site

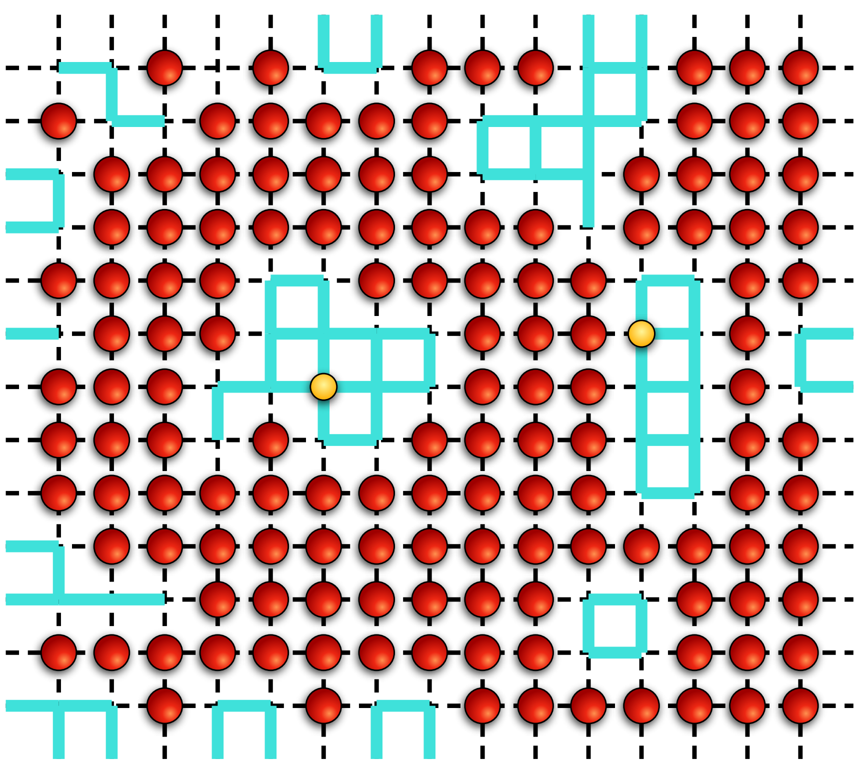
Bosonic correlation function

$$\langle \psi_{x,a}\psi_{x,b}\ \psi_{y,a}\psi_{y,b}\rangle \;=\; \int [d\overline{\psi} d\psi]\ \mathrm{e}^{-S}\ \psi_{x,a}\psi_{x,b}\ \psi_{y,a}\psi_{y,b}$$

vanishes unless x and y are in the same bag!



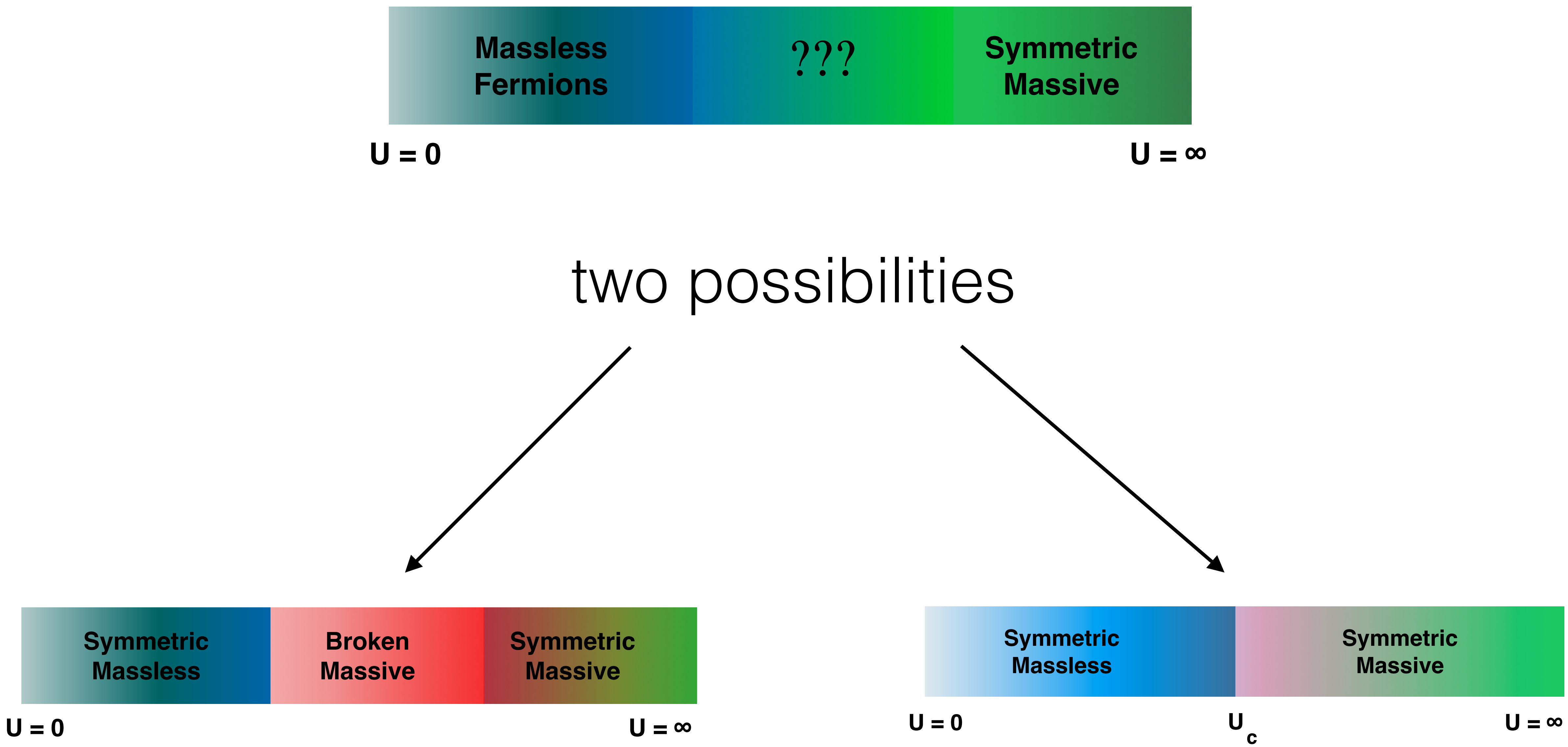
Non-zero!



Zero!

At sufficiently large coupling U
the two point correlation function will exponentially decay!

Need to modify our original phase diagram!



two transitions
(conventional wisdom)

single transition
(exotic phase transition)

Chiral Susceptibility

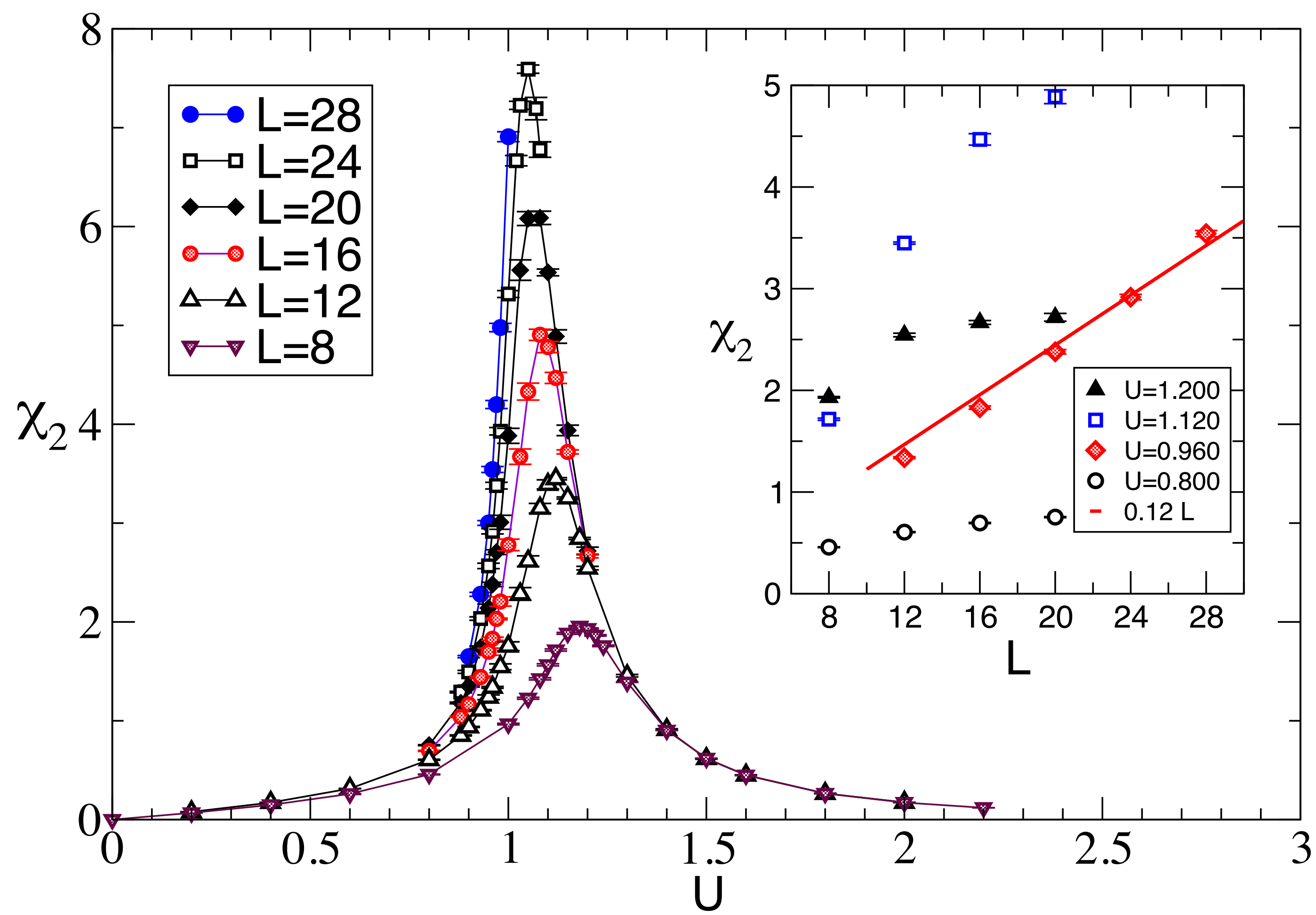
$$\chi_1 = \frac{1}{V}\sum_{x,y} \langle \psi_{x,a}\psi_{x,b}\ \psi_{y,a}\psi_{y,b}\rangle$$

symmetric massless phase and symmetric massive phase

$\chi_1 \sim \text{Const.}$

broken massive phase

$\chi_1 \sim V$



Critical Scaling

Correlation ratio

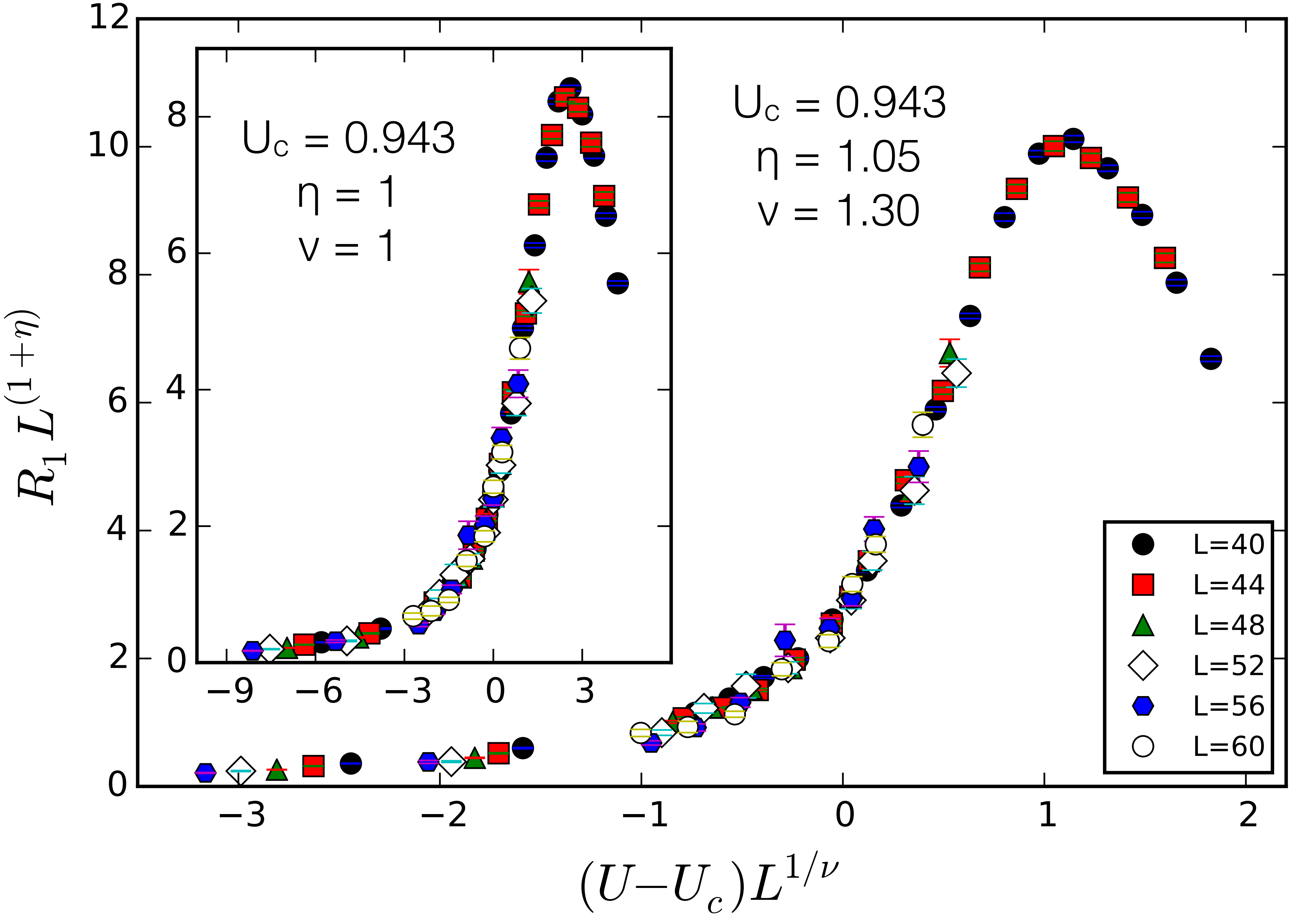
$$R_1(L,U) \;=\; \frac{\langle \psi_{0,a}\psi_{0,b}\;\psi_{L/2,a}\psi_{L/2,b}\rangle}{\langle \psi_{0,a}\psi_{0,b}\;\psi_{1,a}\psi_{1,b}\rangle}$$

Critical Scaling

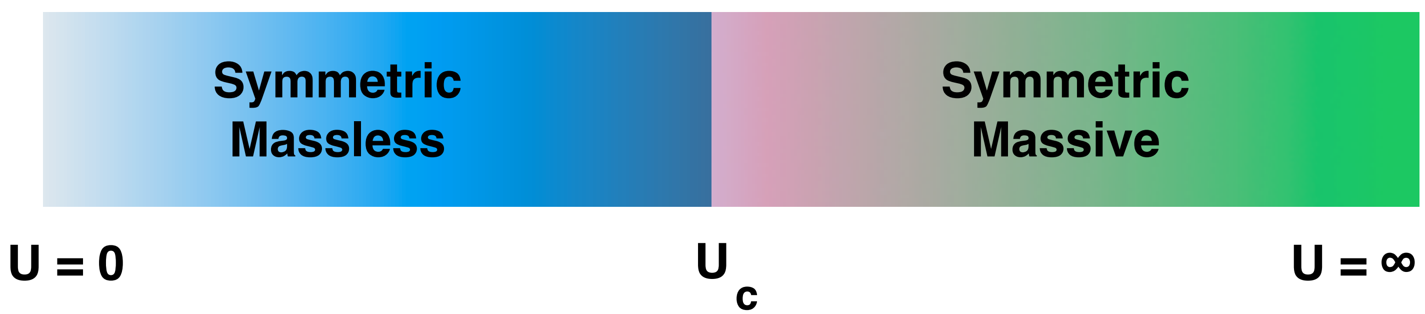
$$R_1(L,U)L^{1+\eta} \;=\; f((U-U_c)\;L^{1/\nu})$$

Our data fits well to this expectation.

Evidence for critical scaling!



Surprising Result!



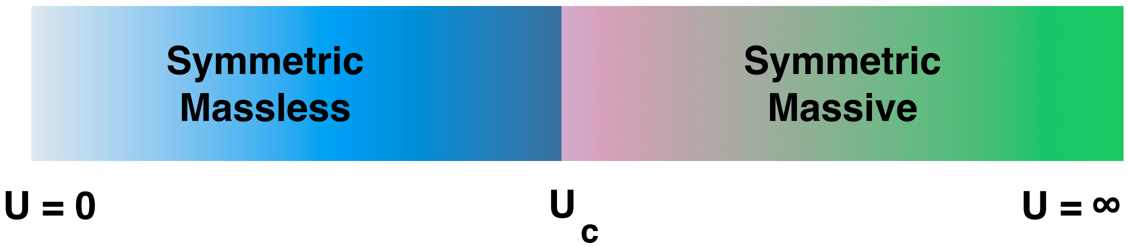
Fermion mass generation is not necessarily related to spontaneous symmetry breaking, but can occur due to dynamics!

Phase transition between two phases with the same symmetries!

Role of Dimension

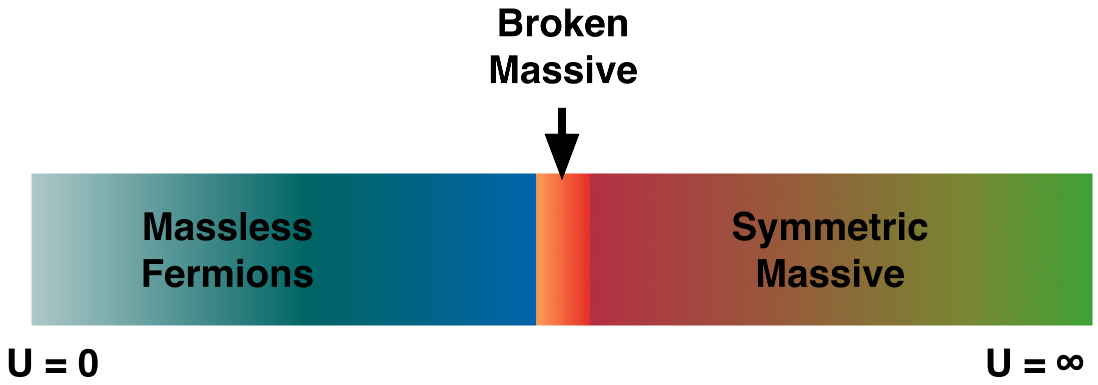
In 3D there is evidence for a single exotic transition

PRD 93 (2016), 081701



In 4D we find evidence for a narrow intermediate spontaneously broken phase

arXiv:1606.06312



In 2D we find evidence for a single asymptotically free (massive) phase

work in progress

Conclusions

Diagrammatic methods offer an alternate approach to Monte Carlo methods.

Several examples already show that they indeed bring new ideas to the table. Still much to learn!

Sign problems always exist in diagrammatic methods!
In some cases they can be solved by resumption methods.
In other cases they may be mild.

They offer a new approach to the problem that must be looked at before being dismissed!