The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

2253-2

Workshop on Synergies between Field Theory and Exact Computational Methods in Strongly Correlated Quantum Matter

24 - 29 July 2011

Deconfined Spinons at 2D Quantum Phase Transition

V.N. Kotov
University of Vermont
Burlington, VT
United States of America

Deconfined Spinons at 2D Quantum Phase Transition

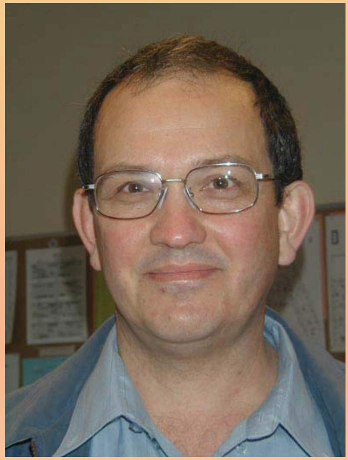
Valeri N. Kotov

(University of Vermont)

ICTP, July 25, 2011

Anders Sandvik (Boston University)

Oleg Sushkov (UNSW, Sydney)



Ref: **“Thermodynamics of Deconfined Bosonic Spinons in Two Dimensions”,**
A.W. Sandvik, V.N. Kotov, and O.P. Sushkov,
Physical Review Letters 106, 207203 (2011)

Outline

1. Conventional (O(3)) versus the Deconfined Criticality Scenario.

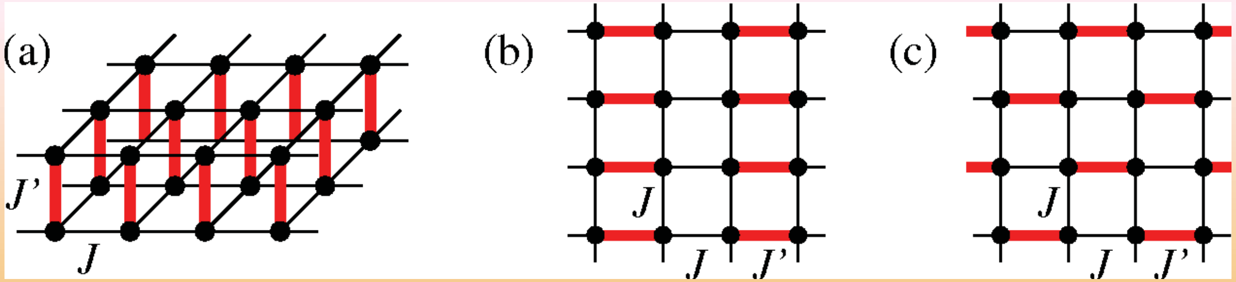
2. Low-energy “phenomenology” near QPT of the J-Q model - Spinon Gas and QMC data fits.

3. Implications for Deconfined Quantum Criticality.

Conventional O(3) transition in 2D antiferromagnets

Theory: Chakravarty, Halperin, Nelson (1989), Chubukov, Sachdev, Ye (1994)

Realized in dimerized S=1/2 Heisenberg models

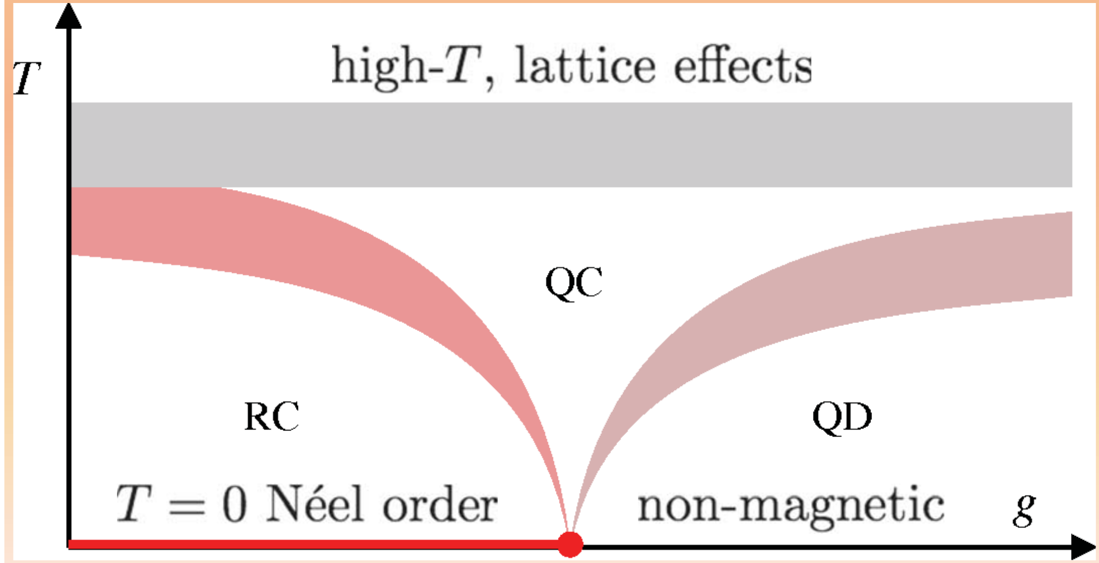


$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle ij \rangle'} \mathbf{S}_i \cdot \mathbf{S}_j$$

Neel - non-magnetic T=0 transition vs **g=J' /J**

- plain singlet-product (+ fluct) state for $g > g_c$

cross-over "phase diagram"



3D O(3) (Heisenberg) universality

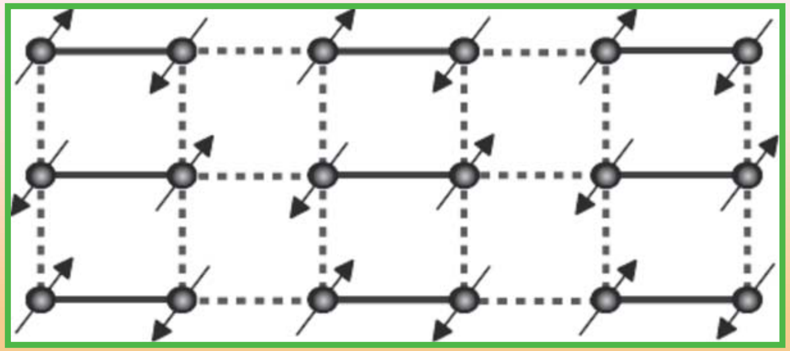
T>0 **quantum-critical regime**

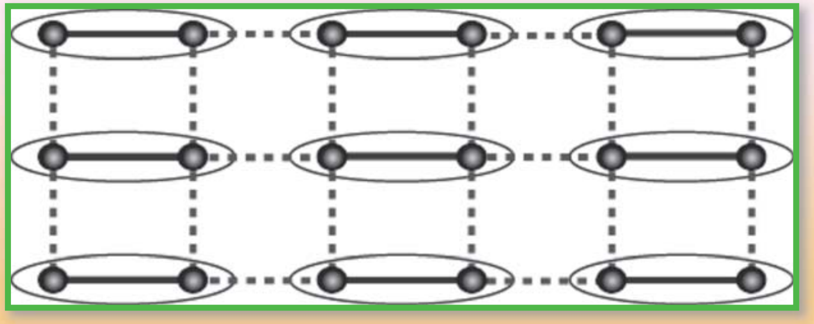
- magnons (S=1) remain as the elementary excitations at the critical point
- dynamic exponent z=1
- scaling behavior:

$$\xi \propto T^{-1}$$
$$\chi \propto T$$
$$C \propto T^2$$

- confirmed by QMC
- some issues remain in (c)

Vector Field $\vec{\varphi} = \eta_i \frac{\vec{S}_i}{S}$; $\eta_i = \pm 1$ on two sublattices





$\varepsilon = ck$

$\left\langle \vec{\varphi} \right\rangle \neq 0$

$\frac{1}{\sqrt{2}}\left(\left| \uparrow \downarrow \right\rangle - \left| \downarrow \uparrow \right\rangle \right)$

$\left\langle \vec{\varphi} \right\rangle = 0$

Néel

Quantum paramagnet

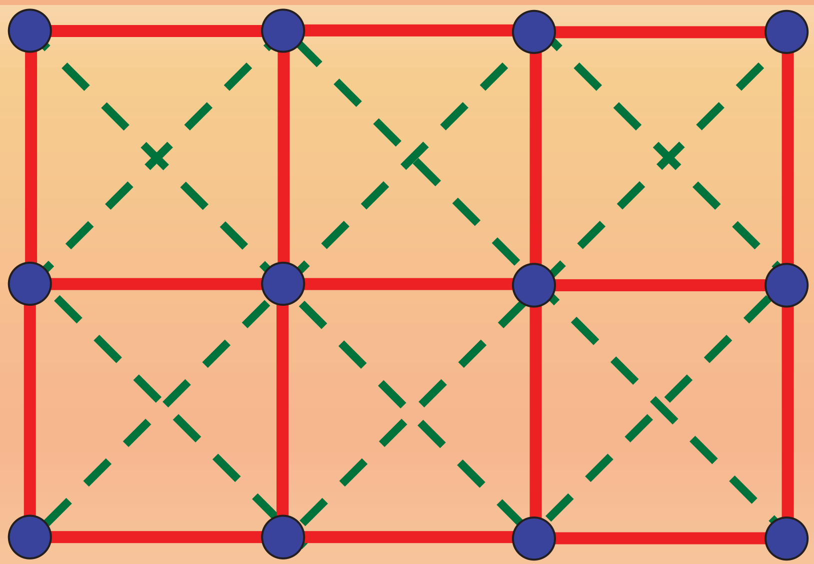
g

g_c

$$S_\varphi = \int d^2x\, d\tau \left[\frac{1}{2}\left(\left(\nabla_x \vec{\varphi} \right)^2 + c^2 \left(\partial_\tau \vec{\varphi} \right)^2 + \left(\lambda_c - \lambda \right) \vec{\varphi}^2 \right) + \frac{u}{4!} \left(\vec{\varphi}^2 \right)^2 \right]$$

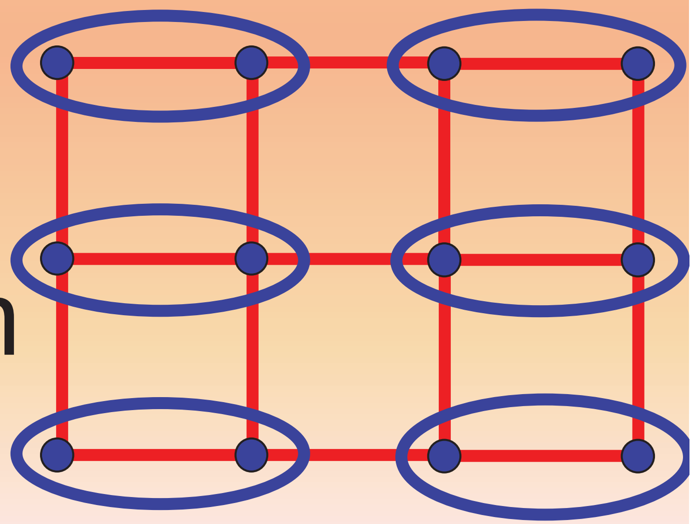
Confinement throughout

Interesting to study Frustration or other Couplings: Destroy Neel order by preserving the full square lattice symmetry, *e.g.* by second-neighbor interactions.



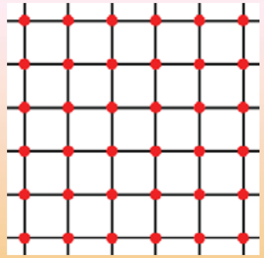
$J_1 - J_2$

Spontaneous dimerization

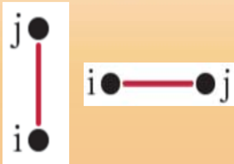


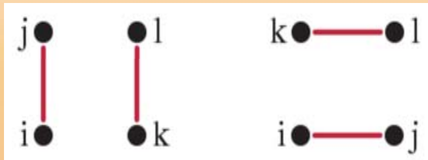
Neel-VBS transition realized in the “J-Q” model (square lattice)

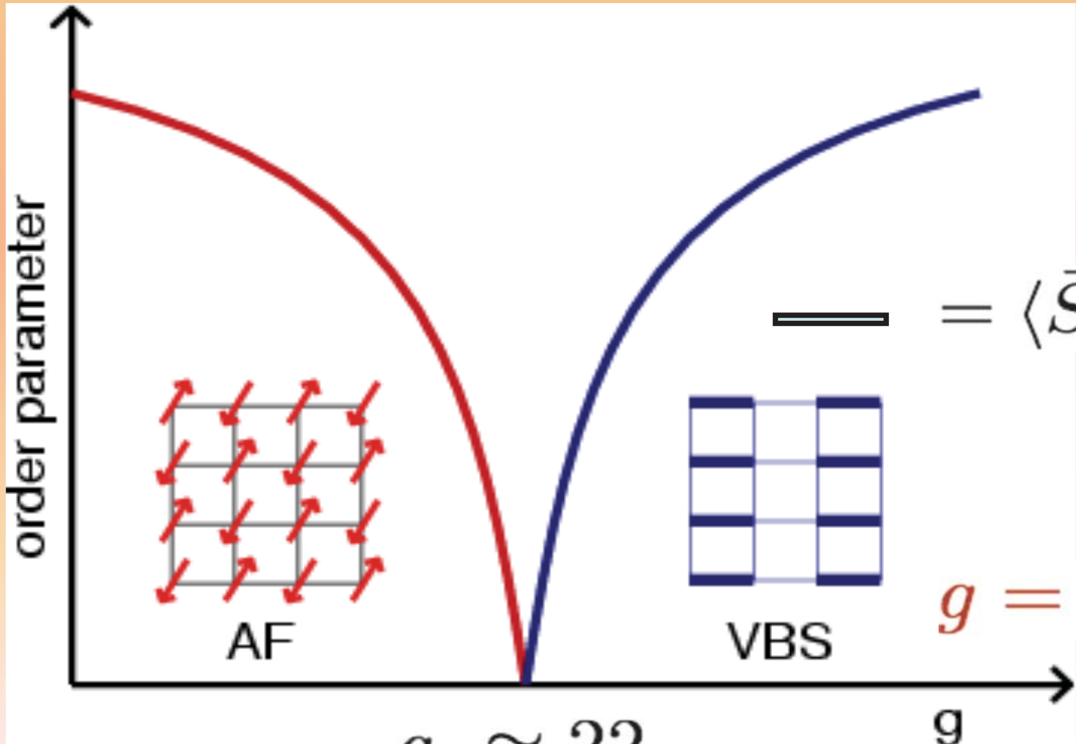
A.W.Sandvik, PRL 98, 227202 (2007)



$$H = J\sum_{\langle ij\rangle} \mathbf{S}_i\cdot\mathbf{S}_j - Q\sum_{\langle ijkl\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4})(\mathbf{S}_k\cdot\mathbf{S}_l-\tfrac{1}{4})$$





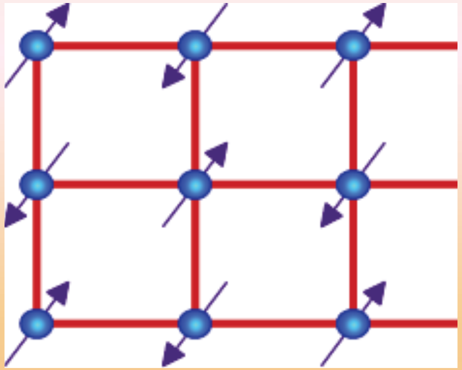


$= \langle \vec{S}_i \cdot \vec{S}_j \rangle$

$g = Q/J$

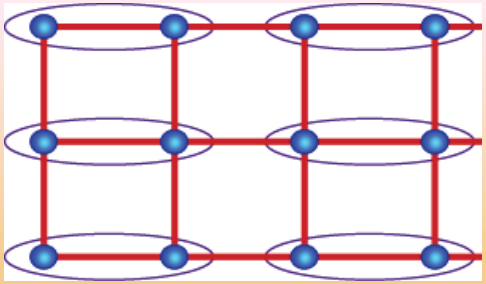
$g_c \approx 22$

Bosonic Spinons: Deconfined Quantum Criticality



Neel order

$$\left\langle \vec{\varphi} \right\rangle \sim \left\langle z_\alpha^* \vec{\sigma}_{\alpha\beta} z_\beta \right\rangle \neq 0$$



Dimer order

$S = 1/2$ spinons z_α confined,

$S = 1$ triplet excitations

g

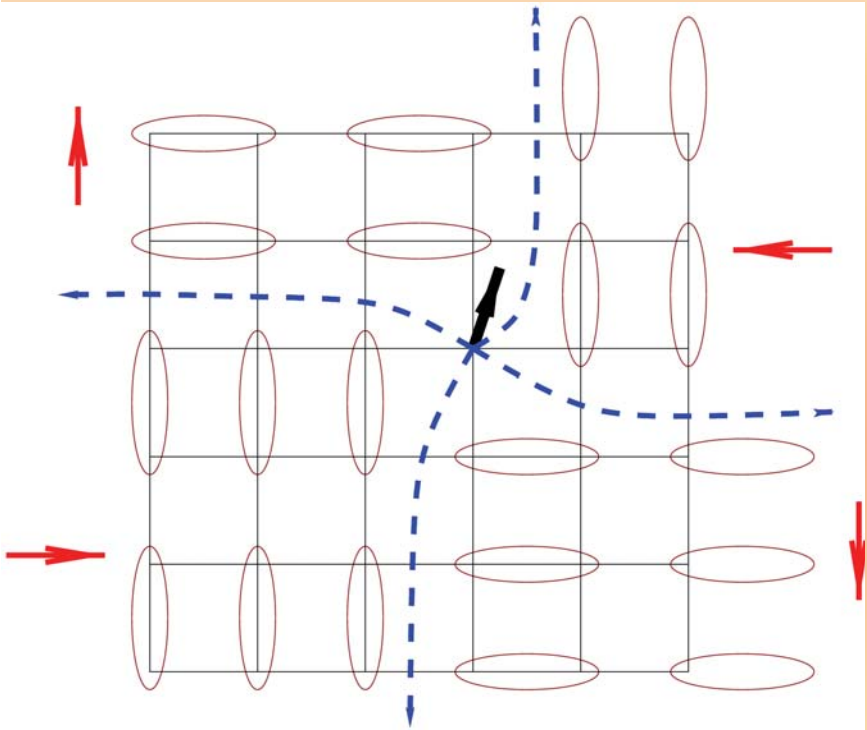
$$\mathcal{S}_{\text{critical}} = \int d^2x d\tau \left[\left|(\partial_\mu - iA_\mu) z_\alpha\right|^2 + r\left|z_\alpha\right|^2 + \frac{u}{2}\left(\left|z_\alpha\right|^2\right)^2 \right.$$

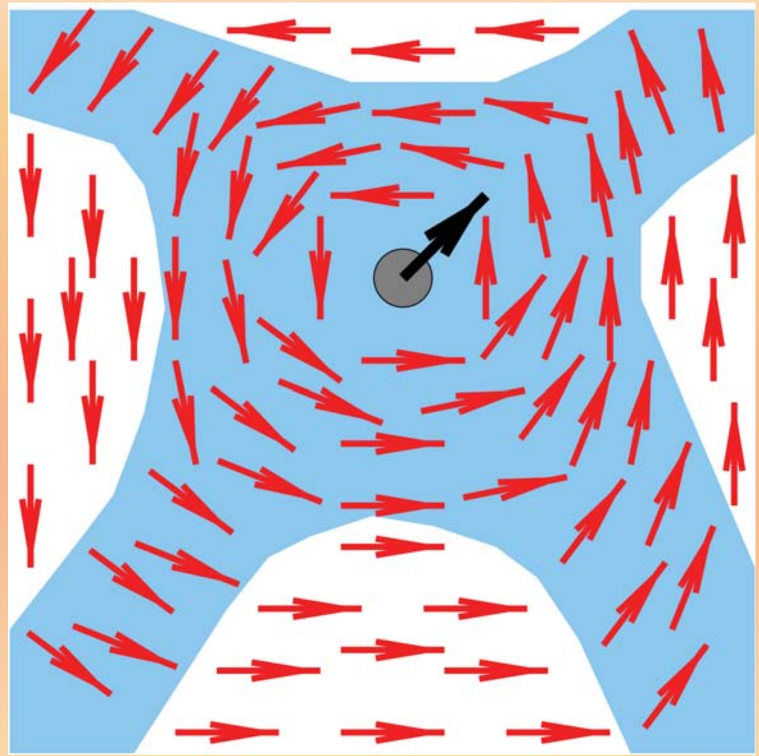
T. Senthil, A. Vishwanath, L. Balents, S. Sachdev , M.P.A. Fisher, *Science* **303**, 1490 (2004).

S. Sachdev

Spinon as unpaired site between dimer patterns
(Z_4 vortex defect)

(Levin,Senthil, 2004)





$$\vec{\varphi} = z^*_{\alpha} \vec{\sigma}_{\alpha\beta} z_{\beta}$$

Near Critical Point

Λ

$$S_{\mathrm{critical}} = \int d^2x d\tau \left[|(\partial_\mu - iA_\mu) z_\alpha|^2 \right.$$

$$\vec{\varphi} = z^*_\alpha \vec{\sigma}_{\alpha\beta} z_\beta$$

CP(N-1); N=2 is physical case

- Phase mode $\Rightarrow$ "Photon" (U(1) gauge field)
- The Spinons (S=1/2) are Bosons (!)

- Dimer order destroyed below the scale

$$\Lambda \propto \xi^{const \times N}$$

(Murthy,Sachdev,1990)

We define:

$$\Lambda \propto \xi^{1+a} \propto \frac{1}{T^{1+a}}$$

$$a \propto N >> 1$$

Spinon confinement length

We find: $a \approx 0.22$

Summary

- **Conventional O(3) Criticality**

  S=1 excitations (magnons)

- **Deconfined Criticality**
  - 2 species of S=1/2 bosons
  - Large confinement scale Λ
  - Need continuous

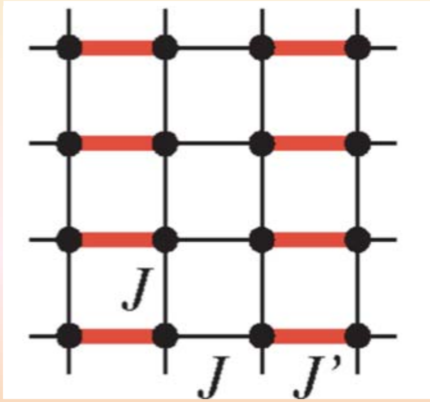
    Neel-Sp. Dimer QPT

Only way to test predictions

→ Experiment

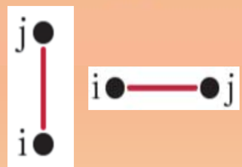
<u>Conventional O(3)</u>

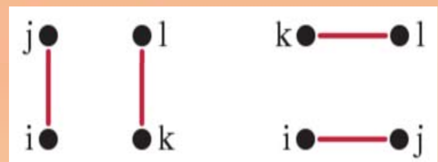
J-J' model



<u>Deconfined (?): J-Q Model ← the only candidate!</u>

$$H = J\sum_{\langle ij\rangle} \mathbf{S}_i\cdot\mathbf{S}_j - Q\sum_{\langle ijkl\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4})(\mathbf{S}_k\cdot\mathbf{S}_l-\tfrac{1}{4})$$



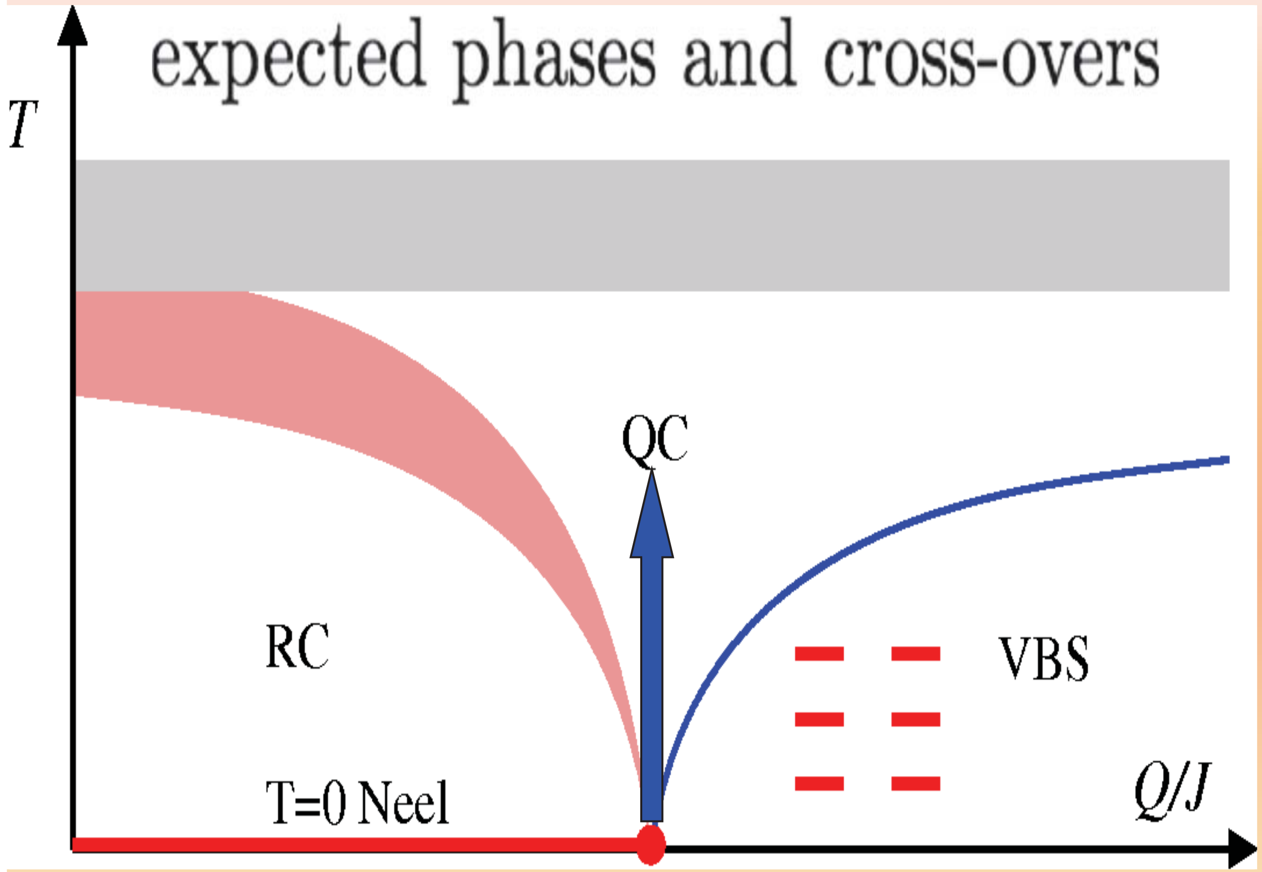


Critical-point estimates

J-J' model: $(J'/J)_c$=1.90948(4), (using J'/J=1.9095)

J-Q model: $(J/Q)_c$=0.04498(3), (using J/Q=0.0450)

Fingerprints of spinons in T>0 Quantum Critical (QC) regime



J-Q QMC results:

Standard QC forms

$$\xi \propto T^{-1}$$

$$\chi \propto T$$

are **weakly violated.** Specific heat obeys the standard form

$$C \propto T^2$$

J-Q Model refs…

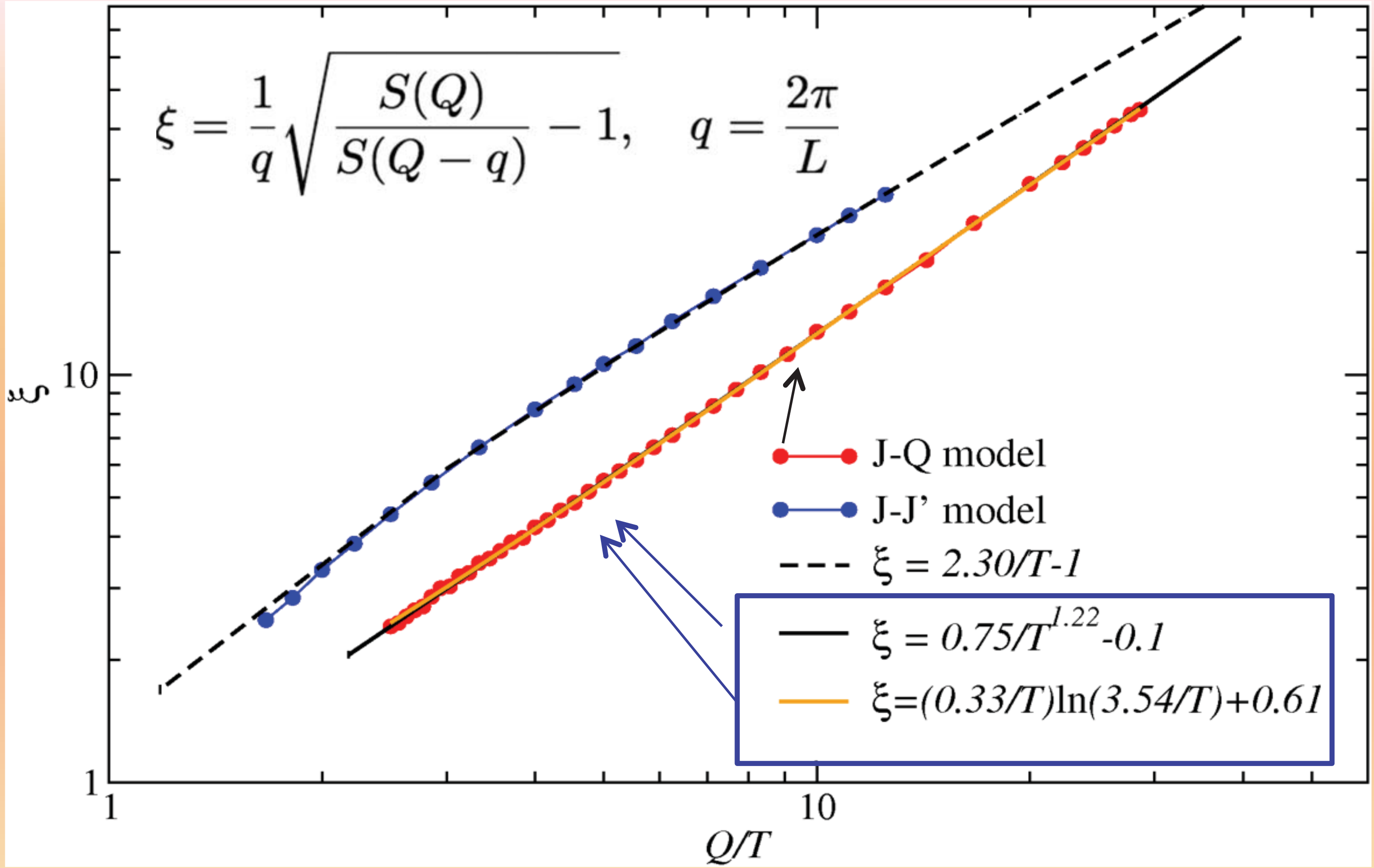
A. Sandvik, PRL **98**, 227202 (2007); **104**, 177201 (2010)
R. Melko, R. Kaul, PRL **100**, 017203 (2008)
A. Sandvik, VNK, O. Sushkov, PRL **106**, 207203 (2011)
R. Kaul and R. Melko, PRB 78, 014417 (2008)
…

Continuous transition between Neel and VBS

Unconventional behavior at Critical Point

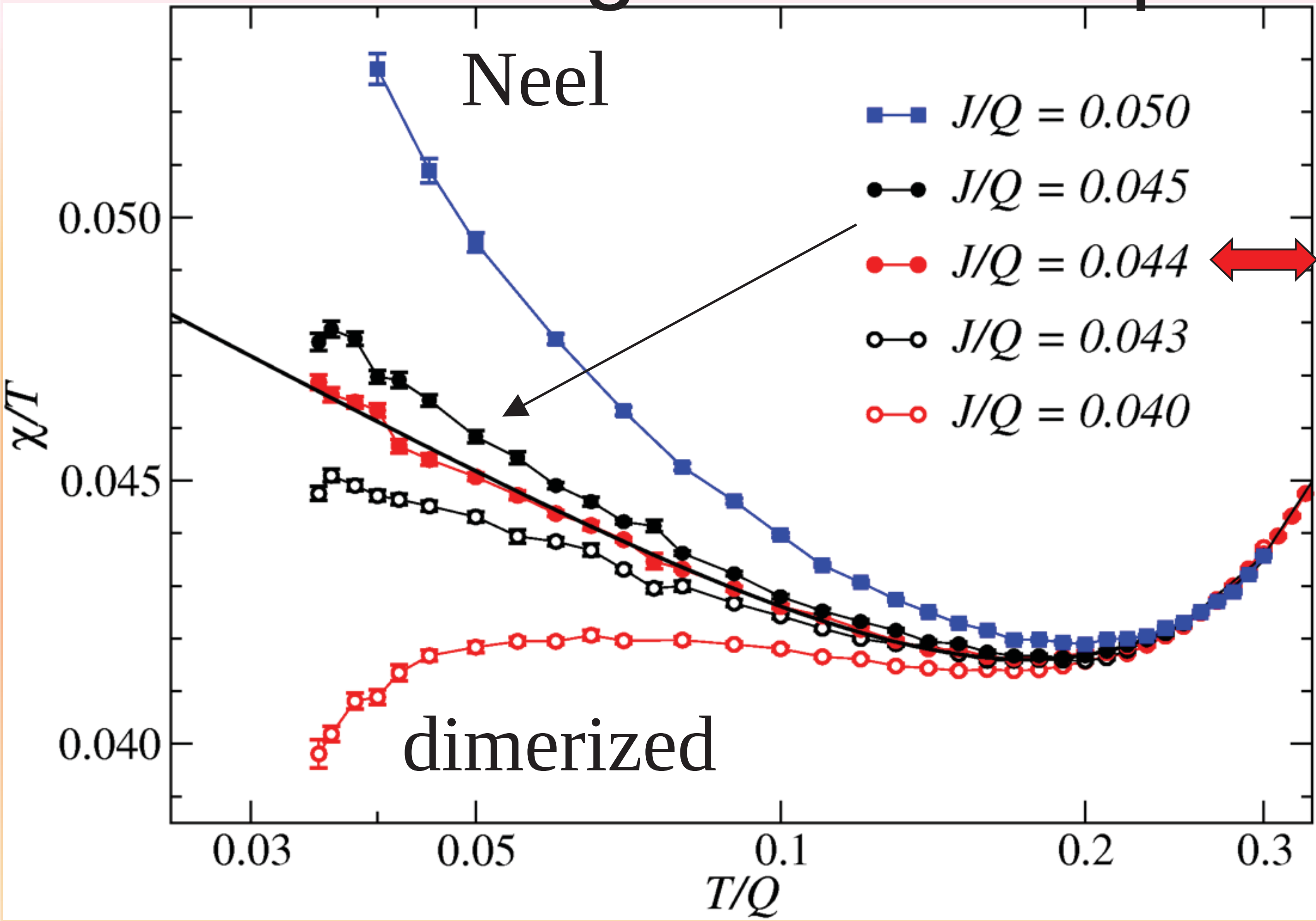
Anomalous Critical Correlation length

- L up to 512; converged to thermodynamic limit for T considered



J-J' model: expected 1/T divergence
J-Q model: faster than 1/T divergence
- logarithmic or power correction (data consistent with either form)

Log Corrections to Critical Scaling in magnetic susceptibility



(J/Q)c=0.044

A.W.Sandvik, PRL 104, 177201 (2010)

$$\chi \sim T[1 + a \ln(1/T)] \quad (L \to \infty)$$

Relationship between the two anomalies?

$$\varepsilon \propto k^z$$

Could the behavior indicate z≠1?

$$\xi \sim T^{-(1/z)}$$
$$\chi \sim T^{2/z-1}$$

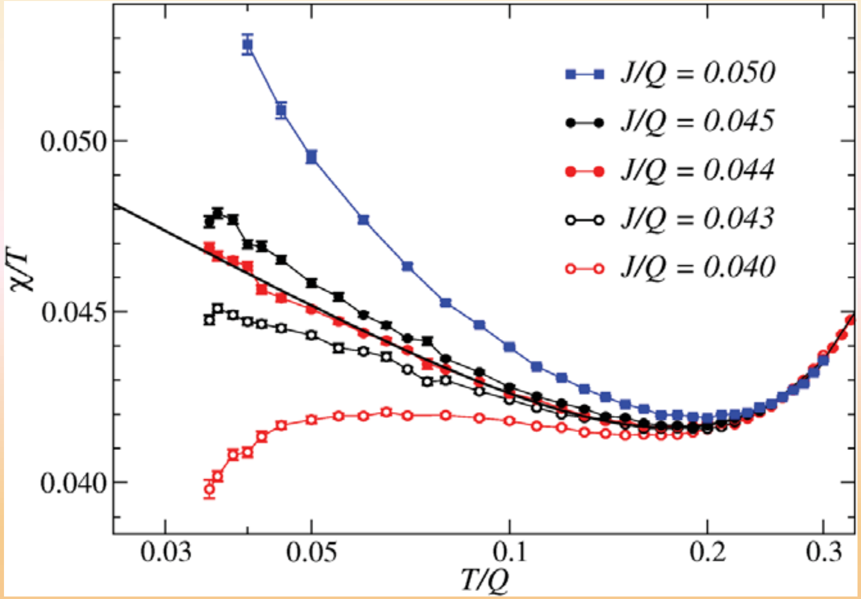
ξ gives z≈0.82 $(\xi \propto 1/T^{1.22})$

- inconsistent with χ(T)

- demands χ/T→0 for T→0

Some unconventional reason

- marginal operator causing logs?



$$\chi \sim T[1 + a\ln(1/T)] \quad (L \to \infty)$$

z=1, but MC measures also spinon component, meaning that ξ and Λ scales are comparable.

$$\Lambda \propto \xi^{1+a} \qquad a = 0.22$$

Spinon Gas Model

- Spinons are non-interacting
- Spinons are de-confined below scale Λ

$$\Lambda \propto \xi^{1+a} \propto \frac{1}{T^{1+a}}, \quad \Delta = T\,(T/c)^{a}$$

Confinement length and Gap

$$\Lambda \propto \xi^{1+a} \propto \frac{1}{T^{1+a}}, \quad \Delta = T\,(T/c)^a$$

$$\epsilon_{\pm}(k) = \sqrt{c^2k^2 + \Delta^2} \pm \mu B \;\equiv \epsilon(k) \pm \mu B$$

$$\mu = 1/2 \text{ (spinons)}$$

Bosons with magnetic moment 1/2

Compare Spinons (S=1/2) and Magnons (S=1)

Gas of non-interacting spinons (S=1/2) or magnons (S=1) at T>0

$$\epsilon_{\pm}(k) = \sqrt{c^2k^2 + \Delta^2} \pm \mu B \equiv \epsilon(k) \pm \mu B$$ (B = magnetic field)

$$\mu = 1/2 \text{ (spinons)}, \quad \mu = 1 \text{ (magnons)}$$

$$\text{Magnetization} = -2\mu^2 F B \int \frac{\partial n}{\partial \epsilon} \frac{d^2k}{(2\pi)^2}$$

$$= \mu^2 F \frac{TB}{4\pi c^2} \int_0^\infty \frac{x\,dx}{\sinh^2[\frac{1}{2}\sqrt{x^2 + (\Delta/T)^2}]}$$

F is a degeneracy factor;
F=2 (spinons/anti-spinons), F=1 (magnons)

Conventional quantum-criticality:
$\Delta/T \rightarrow m \approx 0.96$ (Chubukov & Sachdev 1994)

Using these gaps for spinon (S=1/2) and magnon (S=1) calculations:

$$\Delta_{1/2}/T \;=\; 1/(T\xi) \;=\; (T/mc)^a$$ (***mc*** and ***a*** from J-Q QMC data)

$$\Delta_1/T \;=\; m \;=\; 0.96$$ (Chubukov & Sachdev)

Low-T Critical Magnetic Susceptibility

$$\chi_1 \;=\; (1.0760/\pi c^2)T \longleftarrow \boxed{S=1}$$

$$\chi_{1/2} \;=\; \frac{T}{2\pi c^2}\left[1 + a\ln\left(\frac{mc}{T}\right) + \frac{1}{24}\left(\frac{T}{mc}\right)^{2a}\right]$$

$$\uparrow$$

$$\boxed{S=1/2}$$

Specific heat

$$C_S = (2S+1)F \int \epsilon(k) \frac{\partial n(\epsilon)}{\partial T} \frac{d^2k}{(2\pi)^2}$$

$$C_1 = [36\zeta(3)/5\pi c^2]T^2$$

$$\boxed{S = 1}$$

$$C_{1/2} = \frac{2T^2}{\pi c^2}\left[6\zeta(3) - \left(\frac{T}{c}\right)^{2a}\left[\frac{3}{2} + a + a(1+a)\ln\left(\frac{c}{T}\right)\right]\right]$$

$$\boxed{S = 1/2}$$

Spinons at QCP: $\boxed{\Delta/T = (T/c)^a \to 0}$

Magnetic Susceptibility is infrared divergent:

$$\boxed{\chi_{1/2} = \frac{T}{2\pi c^2}\left[1 + a\ln\left(\frac{c}{T}\right) + \frac{1}{24}\left(\frac{T}{c}\right)^{2a}\right]}$$

for bosons (!); not for fermions

Specific Heat C not singularly affected.

Behavior different from O(3) sigma model (a=0) criticality

Two effects

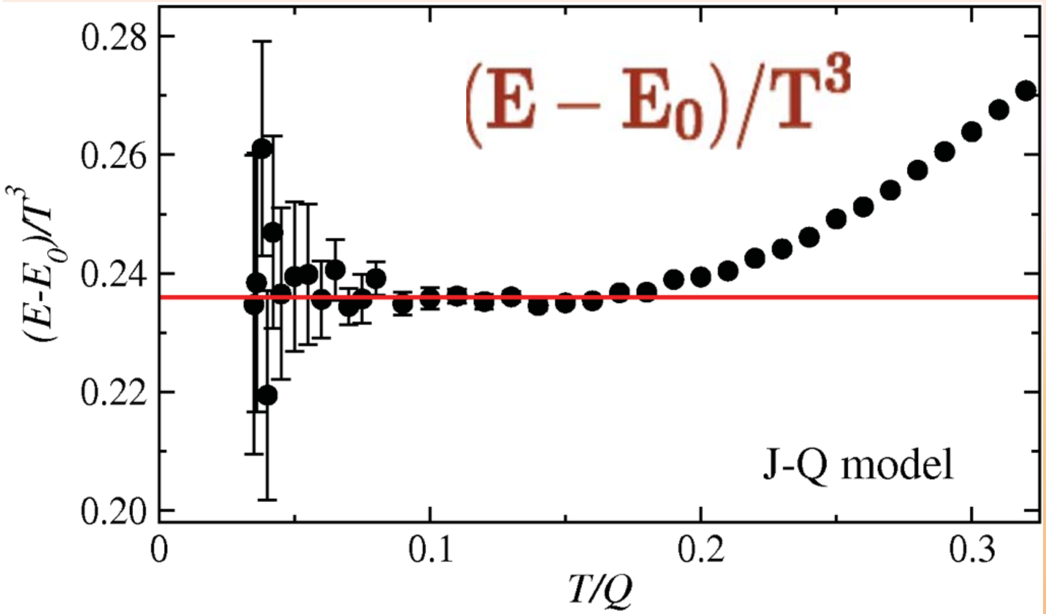
- Critical susceptibility is different for S=1/2

  (reflects spinon magnetic moment and number of species; $\mu^2 F = 1/2$)

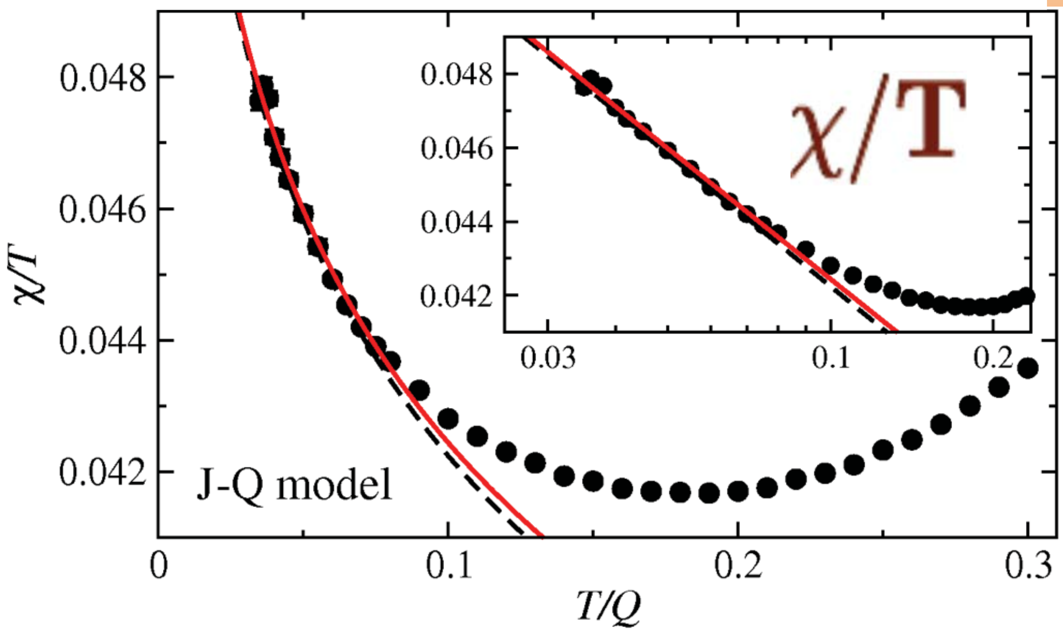
- Violation of critical scaling possible

  (reflects anomalous exponent in confinement scale; bosonic nature of spinons important)

Velocity c is fitted; values from χ/T and C agree within 2%



$$C \propto \left(T/c\right)^2$$



Anomalous exponent

$$a = 0.22$$

$$c = 2.55Q$$

Spinon velocity

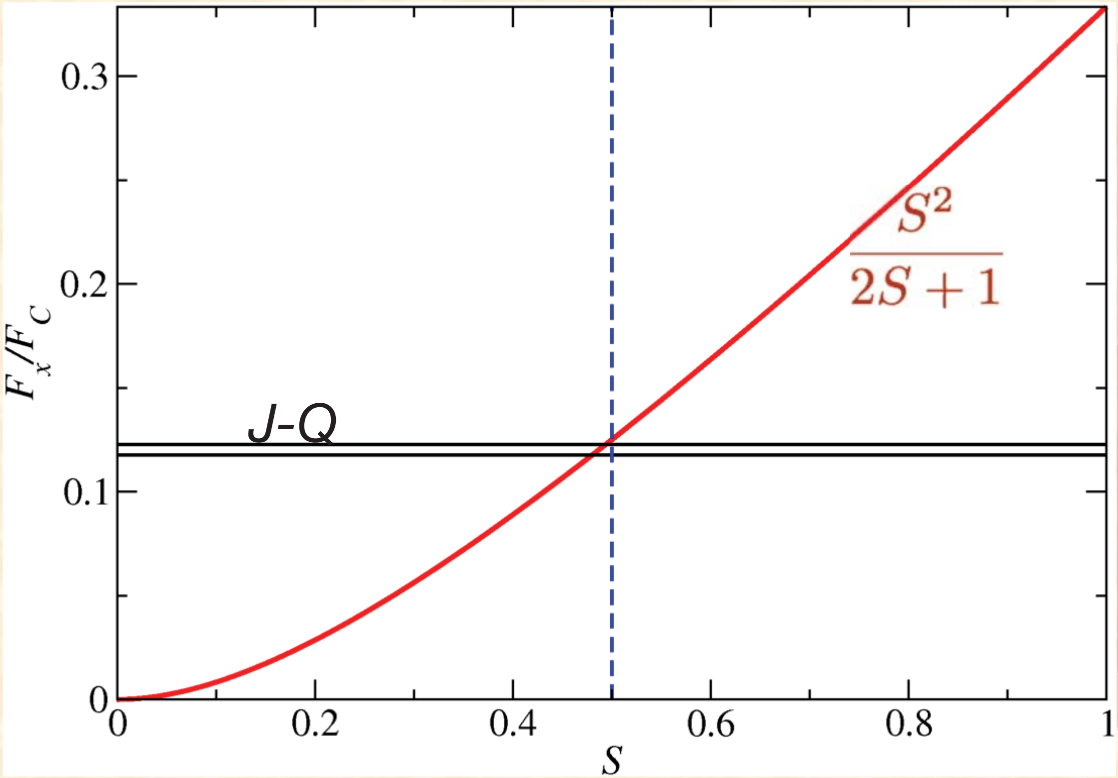
J-Q model: effective spin of the excitations

For spinons, S=1/2, μ =1/2, F=2 (spinon/anti-spinon):

$$F_\chi = \frac{\mu^2 F}{c_\chi^2} \approx 0.074, \qquad F_C = \frac{(2S+1)F}{c_C^2} \approx 0.615 \qquad \begin{aligned} c_\chi &= 2.60 \\ c_C &= 2.55 \end{aligned}$$

Should have **c_χ=c_C.** S≠1/2? For both spinons (S=1/2) and magnons (S=1)

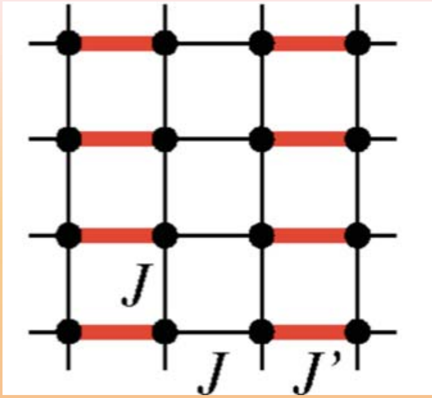
$$\mu = S, \quad \rightarrow \quad \frac{F_\chi}{F_C} = \frac{S^2}{2S+1}$$



The J-Q results are consistent with S=1/2 (spinons) but not consistent with S=1 (magnons)

Independent estimate of the velocity would be good

Conventional O(3)



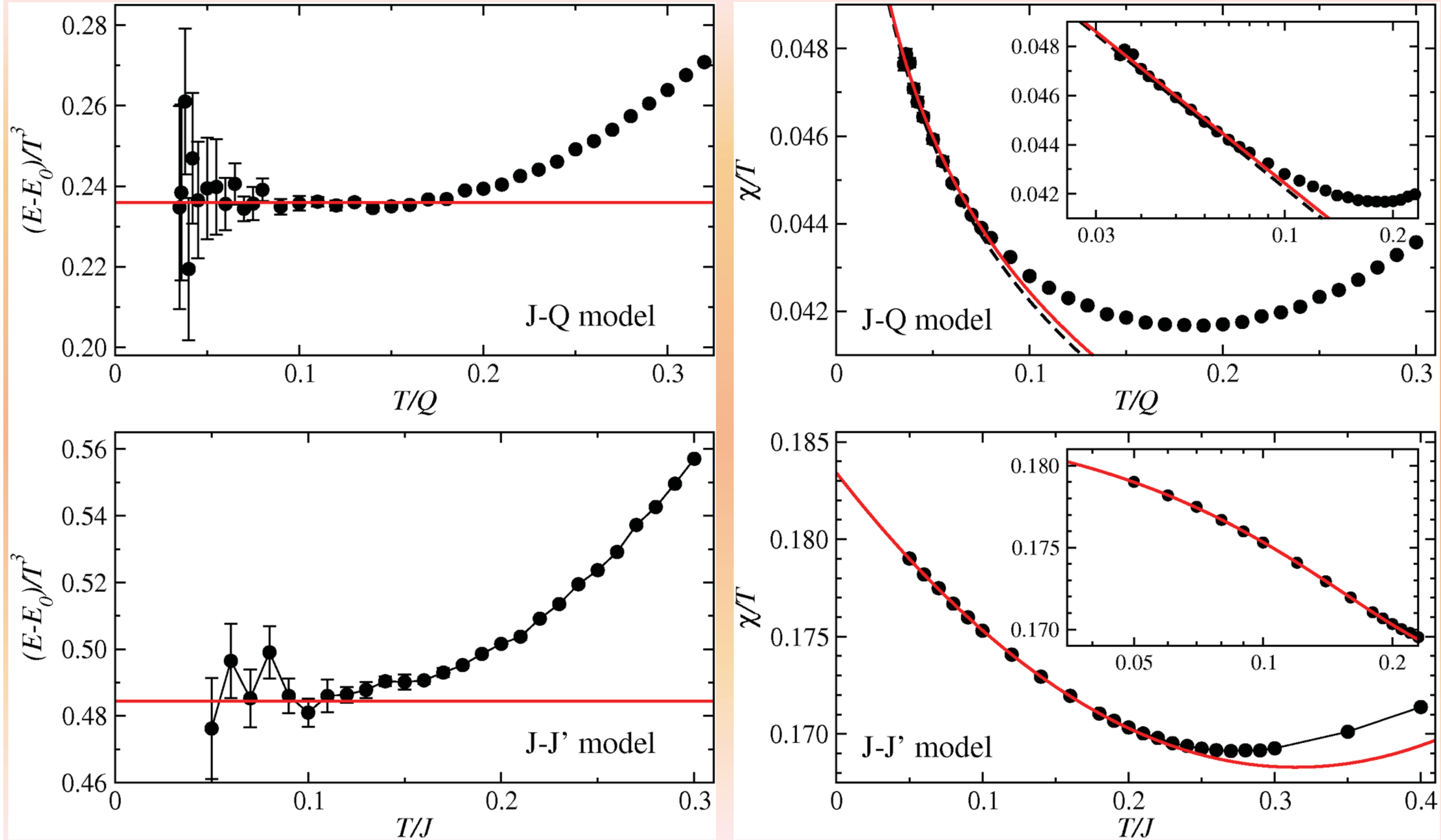
Monte-Carlo data at criticality fit very well by Magnons:

$\mu=1$, Δ/T= const (O(3) sigma model)

QMC data fits: J-J' (magnon forms) and J-Q models (spinon forms)

- **J-J' :** velocity fitted in E/T^3, polynomial fit for χ/T (velocities agree to 2%)
- **J-Q:** velocity is fitted; values from χ/T and C agree within 2%

$$(\mathbf{E}-\mathbf{E_0})/\mathbf{T^3} \qquad \chi/\mathbf{T}$$



Wilson Ratio

Magnons

- $$W_{S=1} = \frac{T\chi}{C} = 0.124$$

Spinons

- $$W_{S=1/2} = \frac{T\chi}{C} = 0.035[1 + a\log(c/T)]$$

Conclusions I

- Strong evidence for bosonic spinons.

★ Log-correction to susceptibility follows from anomalous length scale (within spinon gas approach.)

★ Wilson ratio ($W=T\chi/C$) is weakly divergent.

- This behavior possibly universal characteristic of de-confinement transition (in 2D)

Conclusions II

- In conventional CP(N-1) field theory for large N
  no log-corrections found (but physical N=2)

- Additional probes needed (impurities, magn. field, etc.)

Magnetic Impurity at QCP

Magnons $\chi_{imp} = \tilde{C} / T$

Vojta, Sachdev (2000)

<u>Conjecture:</u> Spinons, with coupling to impurity $J_{imp}\vec{S}_{imp} \cdot (z^*_\alpha \vec{\sigma}_{\alpha\beta} z_\beta)$

- $\chi_{imp} = \frac{C_{Curie}}{T}[1 - f(J_{imp})\log(D/T)], T_K < T < D$
- $\chi_{imp}(T \to 0) = const(?)$

Related work: Florens, Fritz,Vojta (2006)

Physics of screening