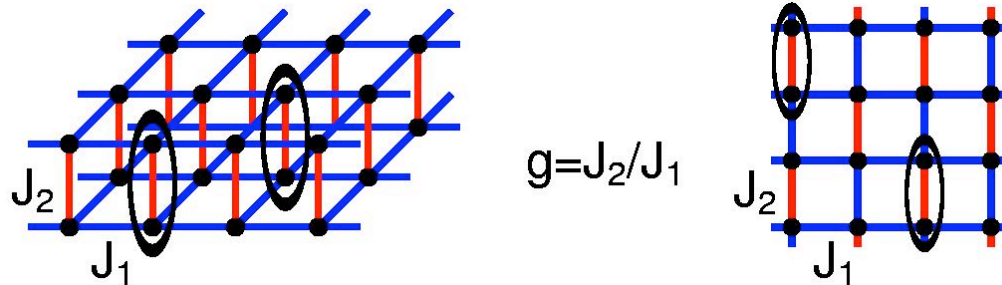


# Quantum criticality in diluted 2D antiferromagnets

Anders W. Sandvik, Boston University

Simulations of dimer-diluted  $S=1/2$  Heisenberg models



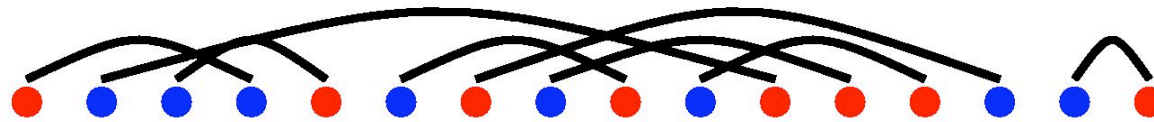
- ⇒ Quantum criticality in the presence of disorder
- ⇒ Geometric/quantum criticality at percolation point

# Background: Random antiferromagnets

1D random  $J > 0$  Heisenberg chain:  $H = \sum_i J_i \vec{S}_i \cdot \vec{S}_{i+1}$

Infinite-randomness fixed point; random-singlet phase:  
Spins form singlets on all length-scales at  $T=0$

Ma, Dasgupta, Hu, 1979; D. Fisher, 1994



Renormalization procedure:  
successive decimation of strongest-coupled pairs

$$\chi \sim \frac{1}{T \ln^2(T)}$$

Dynamic exponent:  $Z = \infty$

$$\omega = k^Z, \Delta_L = L^{-Z}$$

**Dimerized chain:**  $H = \sum_i [J_i + \delta(-1)^i] \vec{S}_i \cdot \vec{S}_{i+1}$

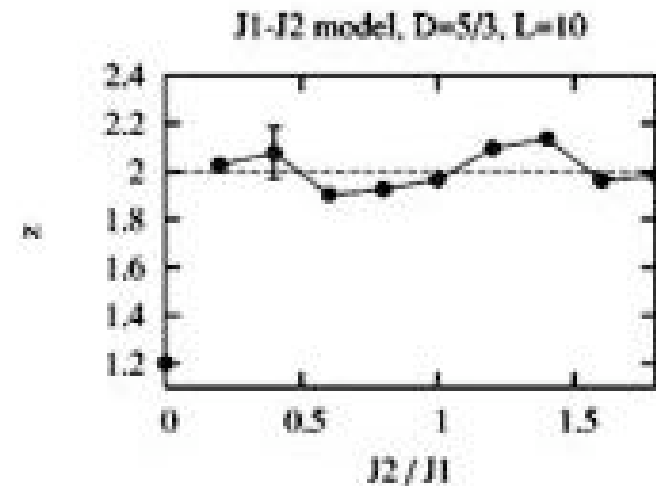
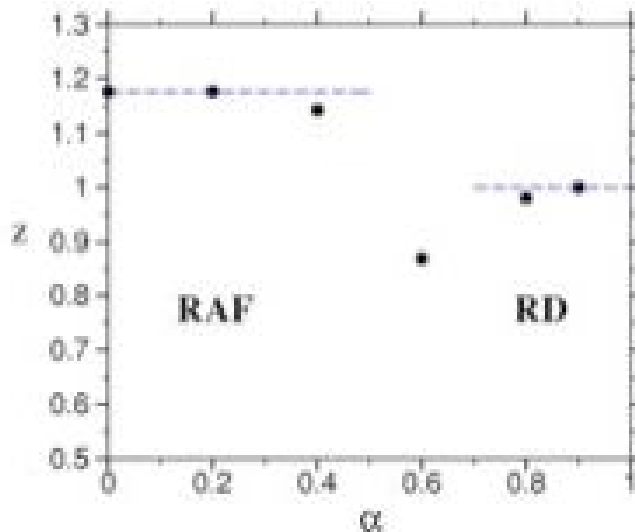
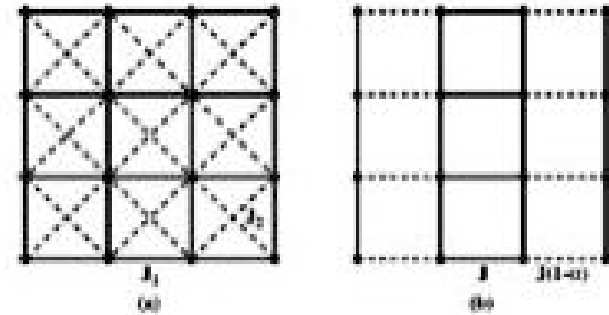
**Griffiths fixed point:**  $Z \propto 1/\delta$   
 Igloi, Juhasz, Rieger (2000)

**2D random transverse Ising model:**  $Z = \infty$

Motrunich, Mau, Huse, D. Fisher (2000); Pich, Young, Rieger, Kawashima (1998)

**2D random J Heisenberg models:**

**RG procedure  $\Rightarrow$  conventional scaling**  
 Lin, Melin, Rieger, and Igloi (2003)



# Site-diluted 2D Heisenberg model

Cuprates: Cu  $\rightarrow$  Zn substitution

Fraction  $p$  of non-magnetic sites

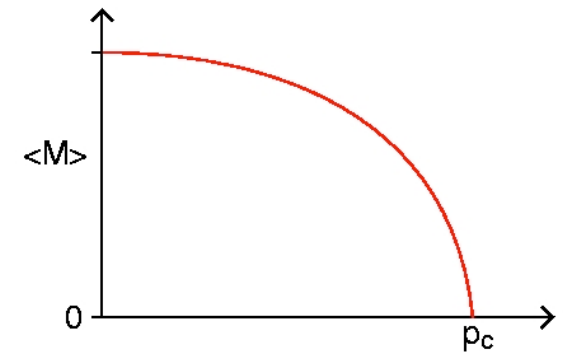
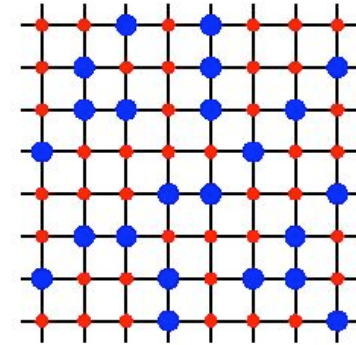
Sublattice magnetization vs  $p$

Is  $p_c$  less than percolation point  $p^* \approx 0.41$ ?

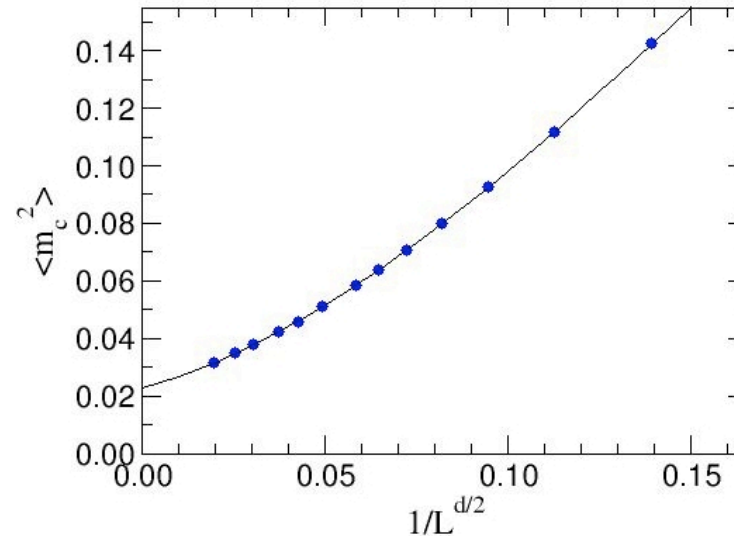
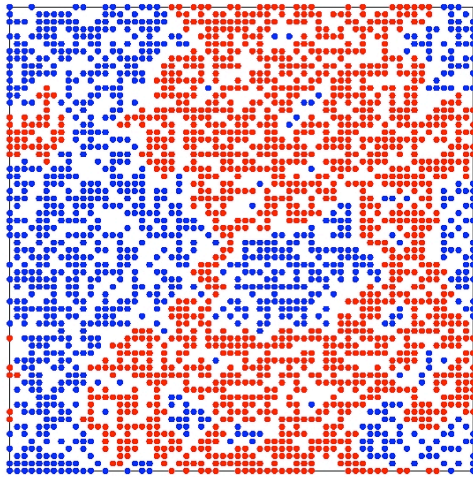
$\Rightarrow$  Kato et al. (2000);  $p_c = p^*$

$\Rightarrow$  Sandvik (2001); percolating cluster ordered

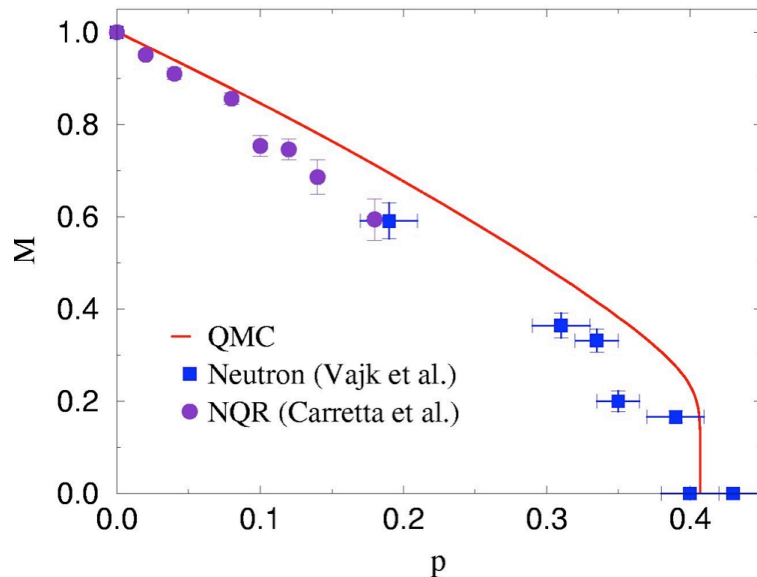
Classical percolation transition



# QMC studies of percolating cluster (d=91/46)



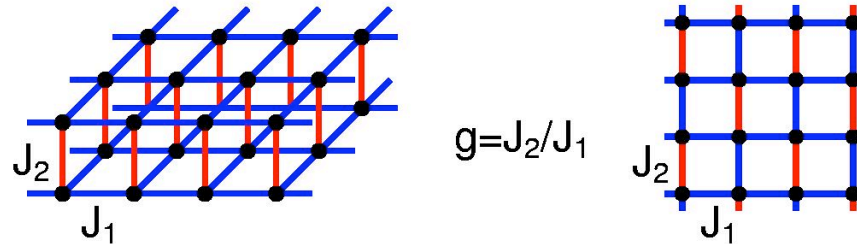
Comparison with neutron scattering;  $\text{La}_2(\text{Zn,Mg})_x\text{Cu}_{1-x}\text{O}_4$



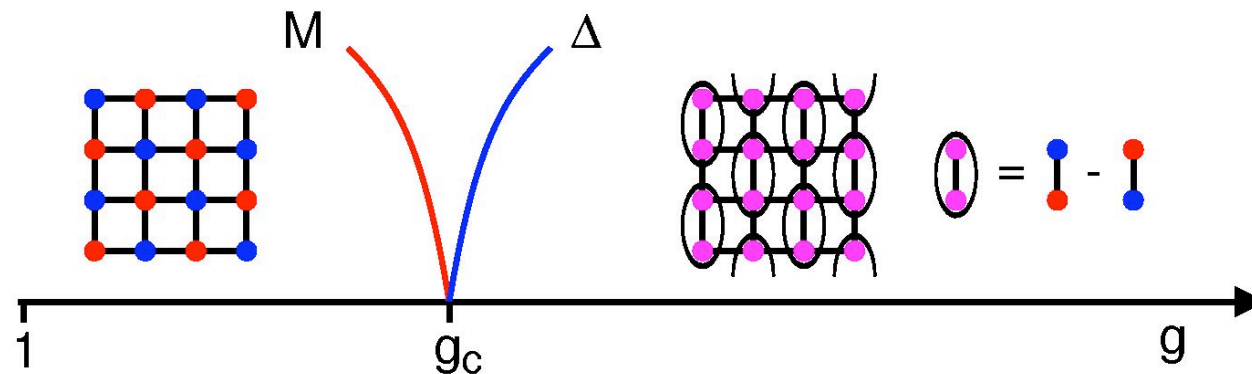
Vajk, Greven, Mang, Lynn, Gehring (2001)

Order slightly suppressed;  
likely other interactions present

# Quantum-criticality in dimerized 2D systems



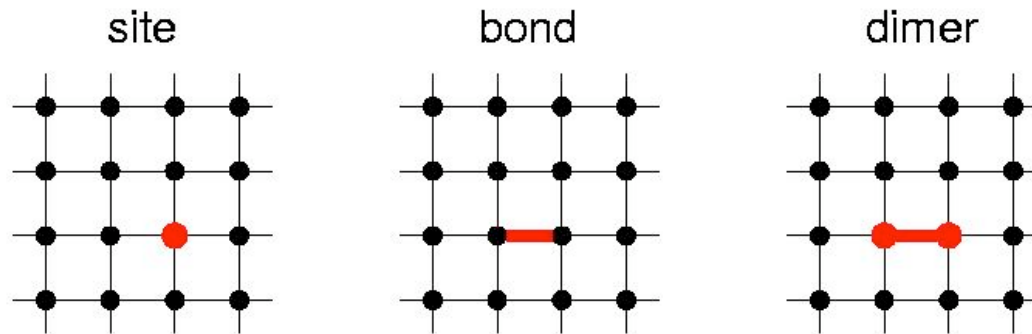
Singlet-formation at strong bonds ("dimers")  $\Rightarrow$  antiferromagnetic to spin-gapped transition



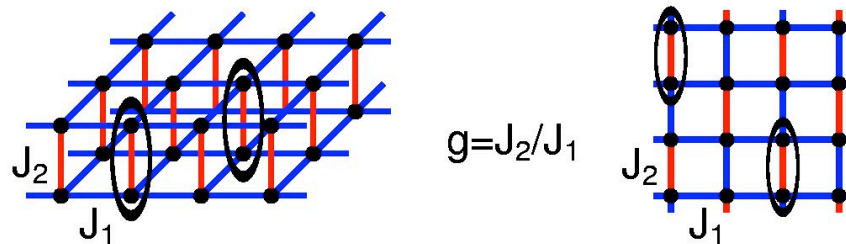
$g_c \approx 2.5$  in both bilayer and single-layer model

# Quantum-critical diluted systems

Unpaired spins in site-diluted gapped system  $\Rightarrow$   
localized moments form; order antiferromagnetically  $\Rightarrow$   
no quantum-critical point



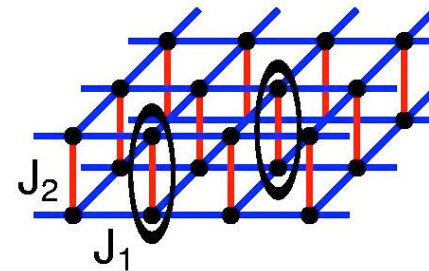
Dimer-diluted models:



# Bilayer model

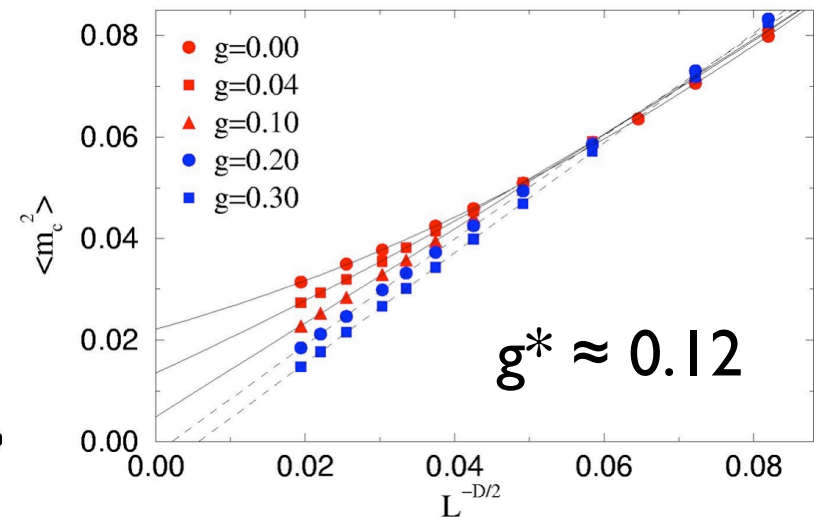
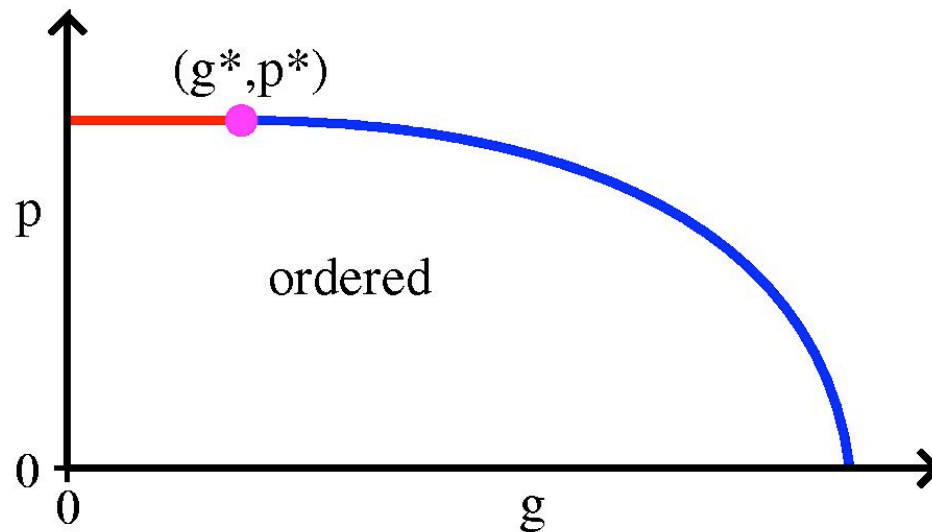
Sandvik (2002); Vajk, Greven (2002)

Sknepnek, Vojta, Vojta (2004)



$$g = J_2/J_1$$

Geometric percolation transition expected for  $g < g^*$



Disorder relevant at transition for  $g > g^*$ ,  $p < p^*$   
(Harris criterion;  $\nu < 2/d$ )

Confirmed in simulations of 3D classical model  
with columnar defects (Sknepnek, Vojta, Vojta);  $Z = 1.310(6)$



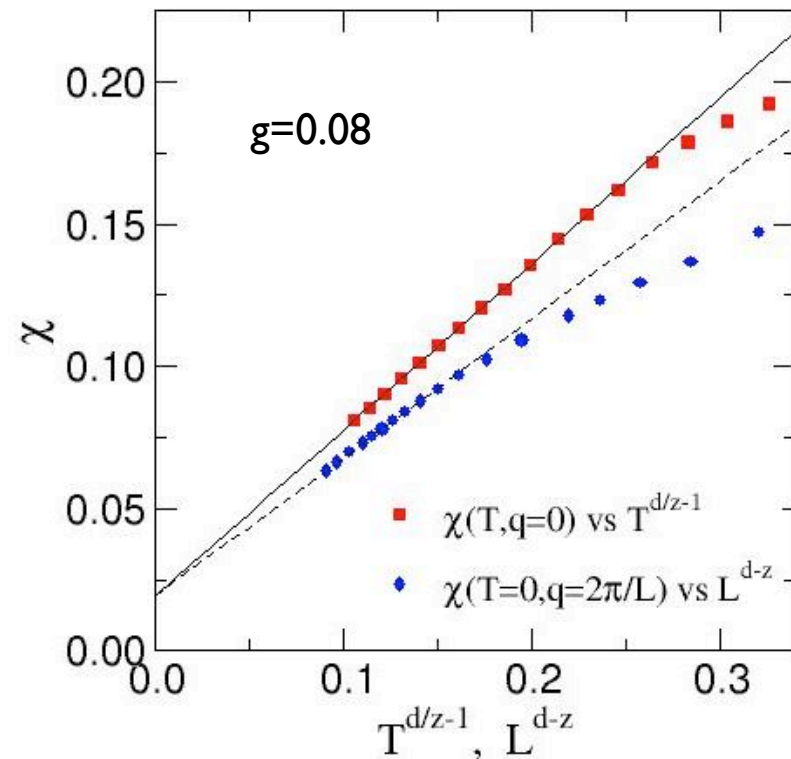
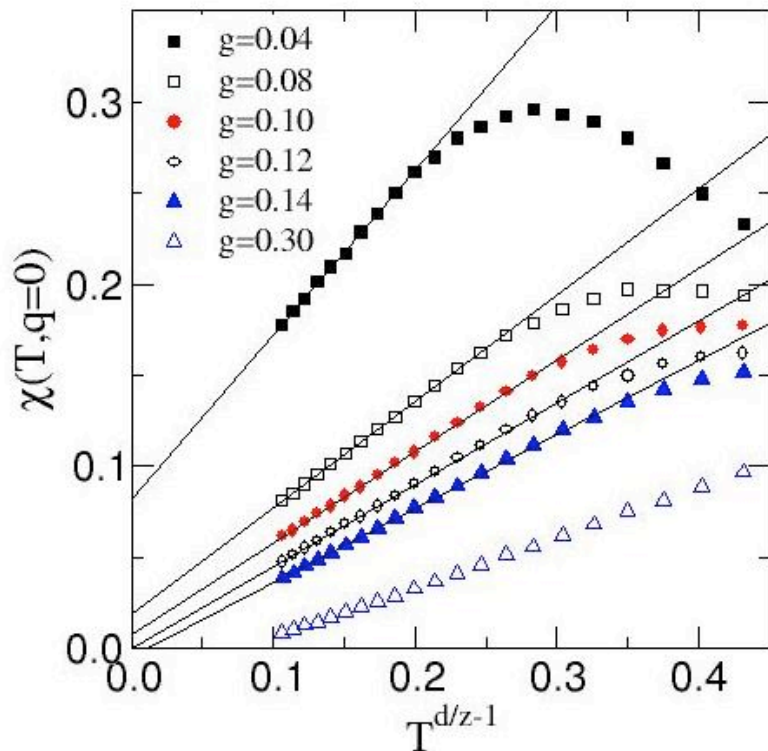
## Uniform magnetic susceptibility

$T > 0$  quantum-critical form:  $\chi = a + bT^{d/z-1}$

$T=0$ ;  $\chi = 0$  for finite system. Use  $\chi(q \rightarrow 0^+)$

$$\xi \sim T^{-z}; \chi = a + b\xi^{z-d} \quad \xi \rightarrow L$$

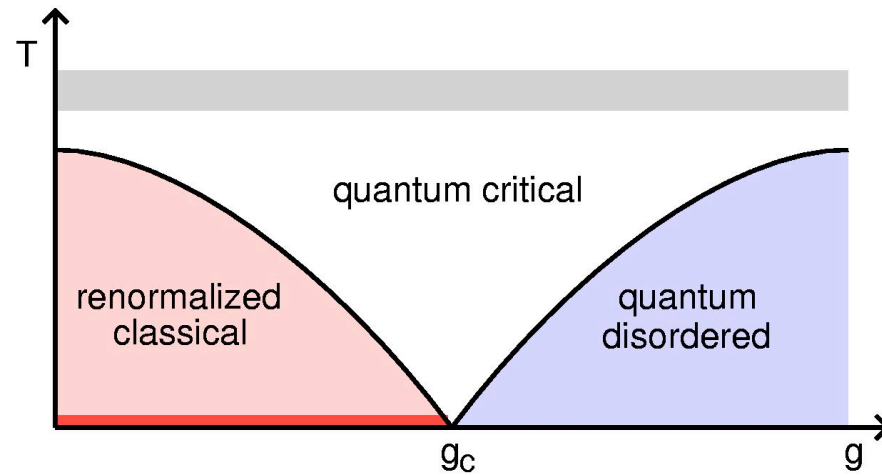
$$\chi(T = 0, q \rightarrow 0^+) = a + bL^{z-d}$$



$$Z=1.36(2)$$

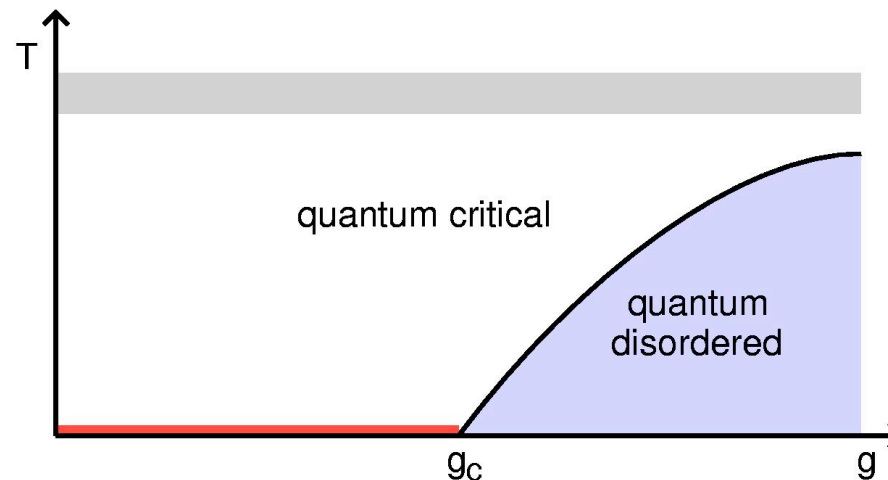
# No sign of quantum-critical to renormalized classical cross-over

Pure 2D antiferromagnet (Chakravarty, Halperin, Nelson)



Low- $T$  cross-overs controlled by spin-stiffness/gap

Conjecture: Stiffness = 0 on percolating cluster; no RC cross-over

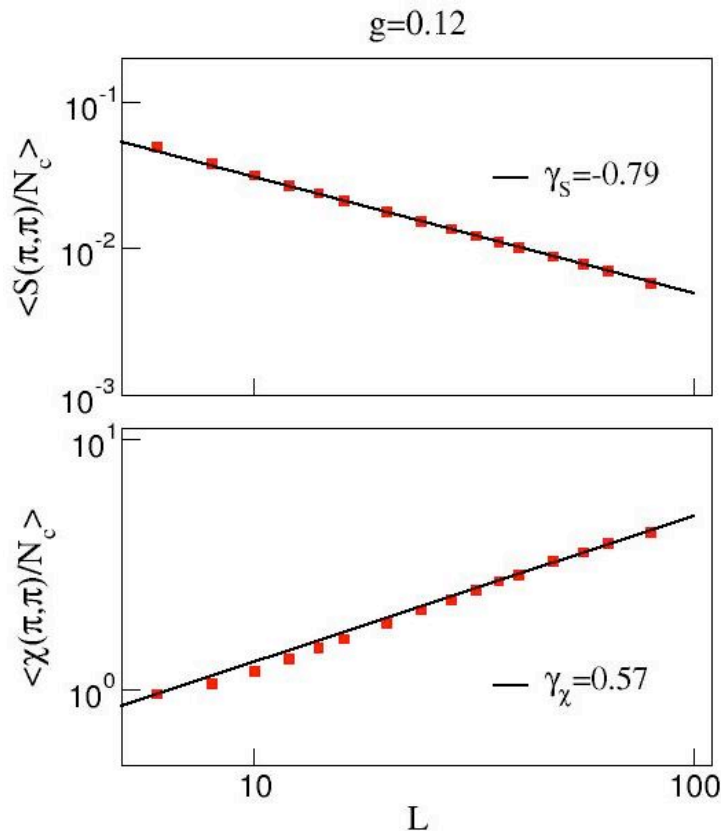


## Check of scaling (Z) using antiferromagnetic quantities

$$q = (\pi, \pi)$$

$$S(q) = \langle S_{-q}^z S_q^z \rangle = \int d\omega S(q, \omega) \sim L^{1-\eta}$$

$$\chi(q) = \int_0^{1/T} d\tau \langle S_{-q}^z(\tau) S_q^z(0) \rangle = \int d\omega \frac{1}{\omega} S(q, \omega) \sim L^{1+z-\eta}$$

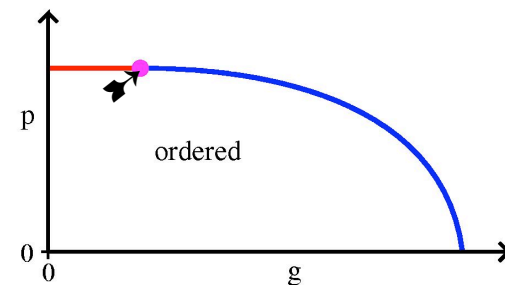


$$1 - \eta = \gamma_S$$

$$1 + z - \eta = \gamma_\chi$$

Data at g close to g\* consistent with

$$z = \gamma_\chi - \gamma_S \approx 1.36$$



Correlation length measured by neutron scattering in  
 $\text{La}_2(\text{Zn,Mg})_x\text{Cu}_{1-x}\text{O}_4$

Vajk, Greven, Mang, Lynn, Gehring (2001)

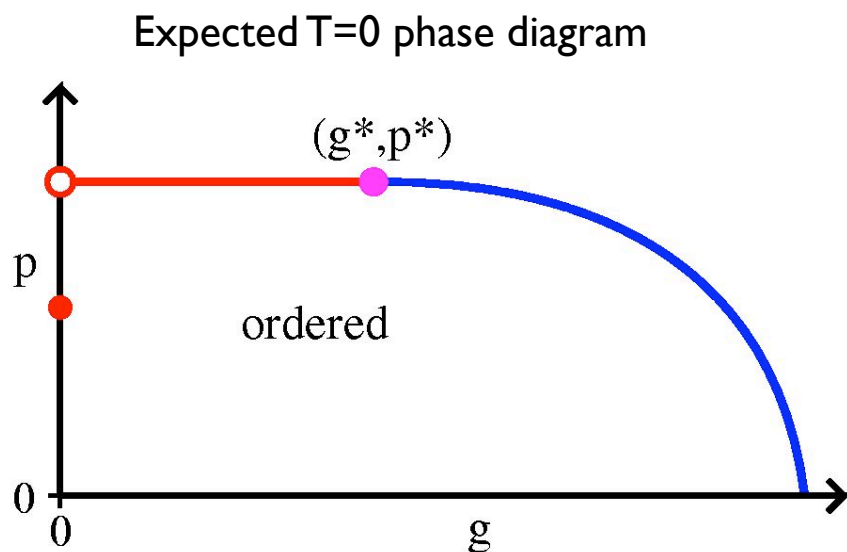
Close to percolation:  $\xi \sim 1/T^z, z \approx 1.4$

Could this be due to multi-critical point ( $g^*, p^*$ )  
in extended parameter space?

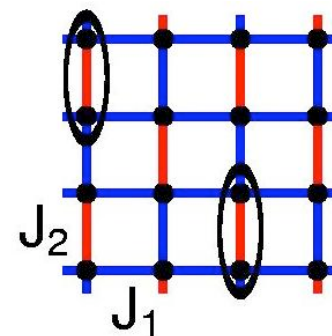
How universal is the behavior found for the  
diluted bilayer antiferromagnet?

Can similar behavior be observed in a single layer?

# Single layer with staggered dimers

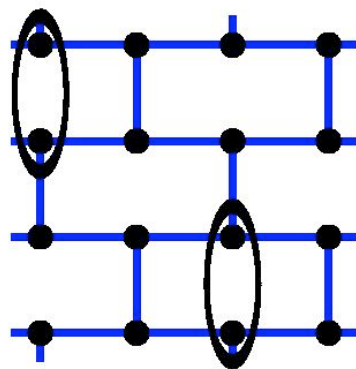


$$g = J_2/J_1$$



Dimers form triangular lattice;  $p^* = 1/2$

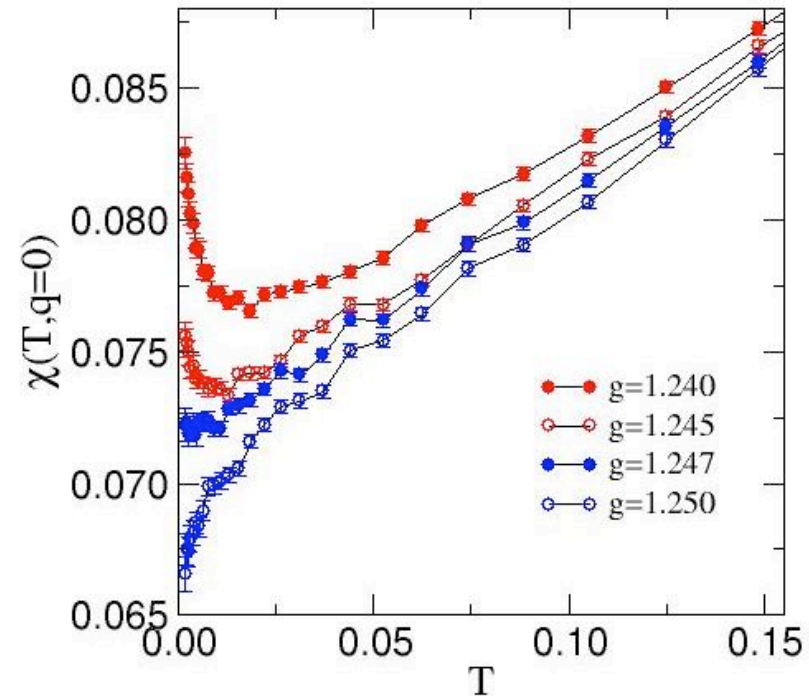
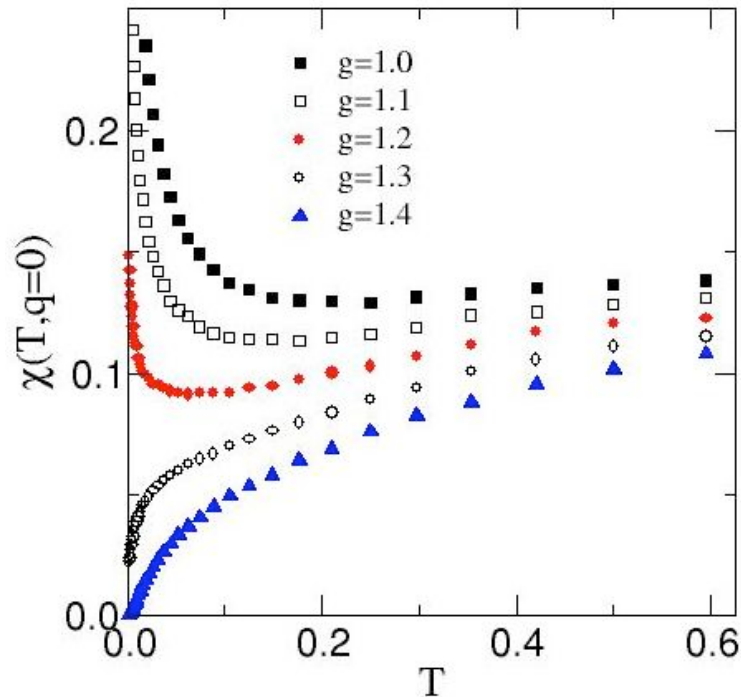
Brick-wall lattice when  $g=0$ ; different percolation point



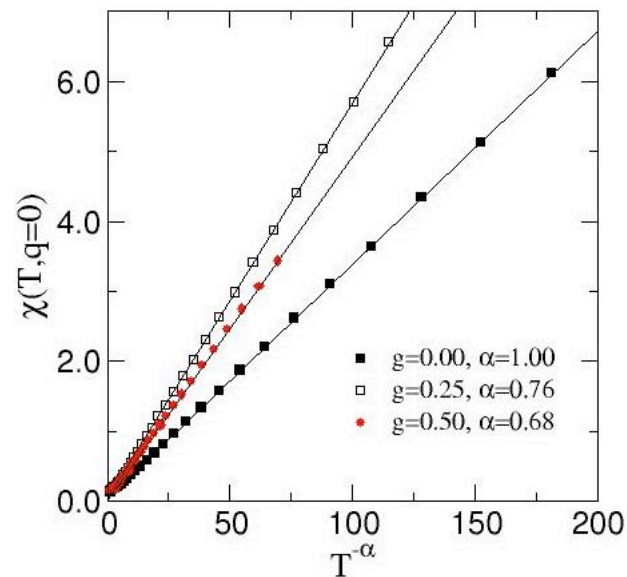
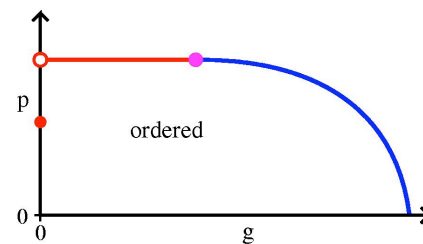
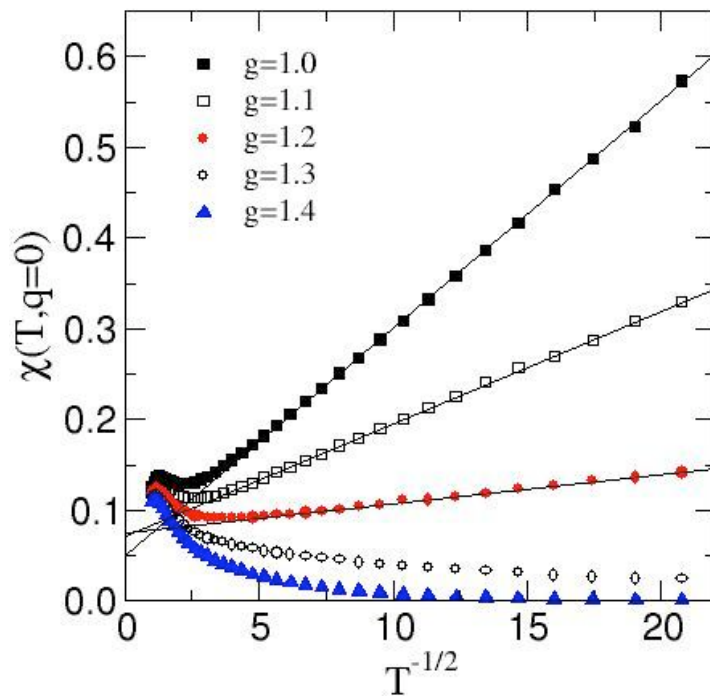
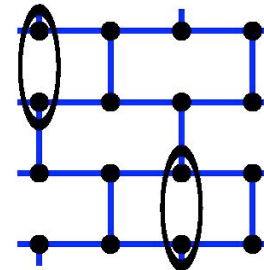
$$P^*(g = 0) \approx 0.29$$

## Uniform susceptibility at $p^*(g>0)$

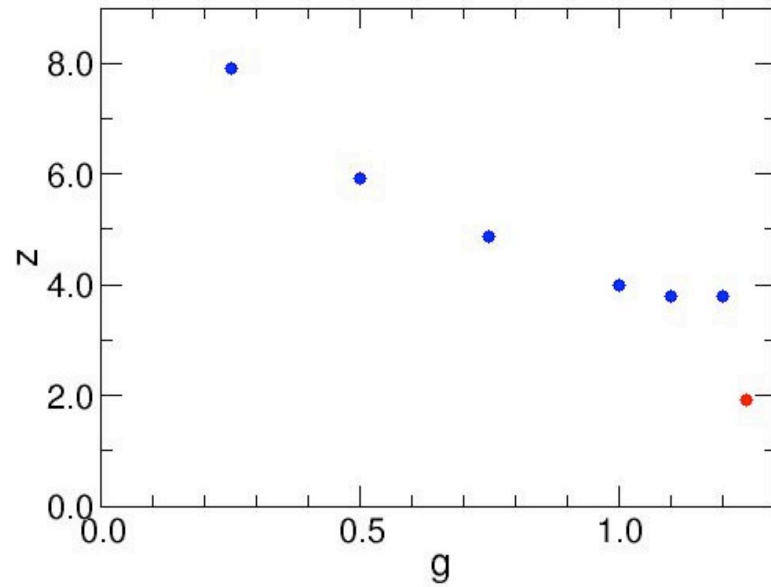
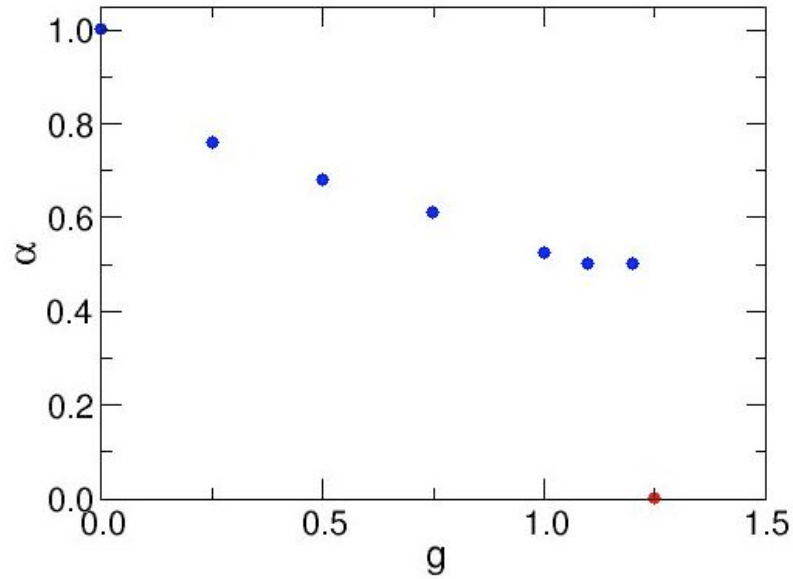
- Indicates critical point;  $g_c \approx 1.247$
- Finite susceptibility at critical point
- Divergent susceptibility for  $g < g_c$



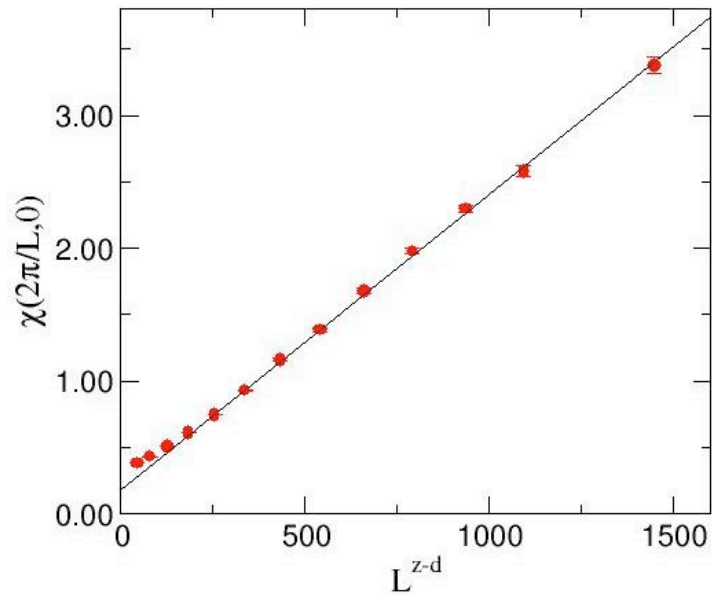
- Divergence follows closely  $T^{-1/2}$  for  $g > 1$
- Faster divergence for smaller  $g$
- Curie form for  $g=0$ , due to “broken clusters”



Extracting z using the form  $\chi = aT^{-\alpha} = aT^{d/z-1}$

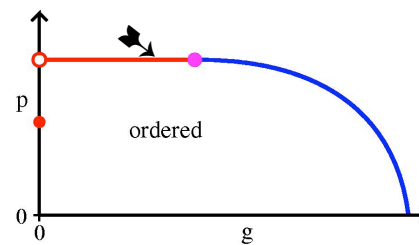


g=1.0



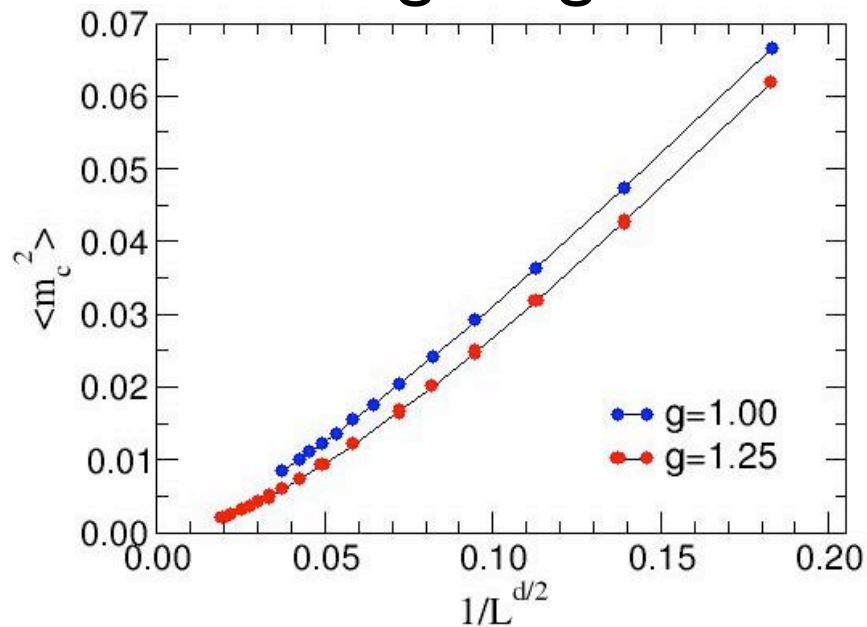
T=0 scaling consistent with T>0 scaling

$$\chi(q \rightarrow 0^+) \sim L^{z-d}$$

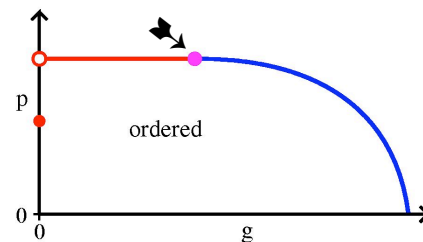




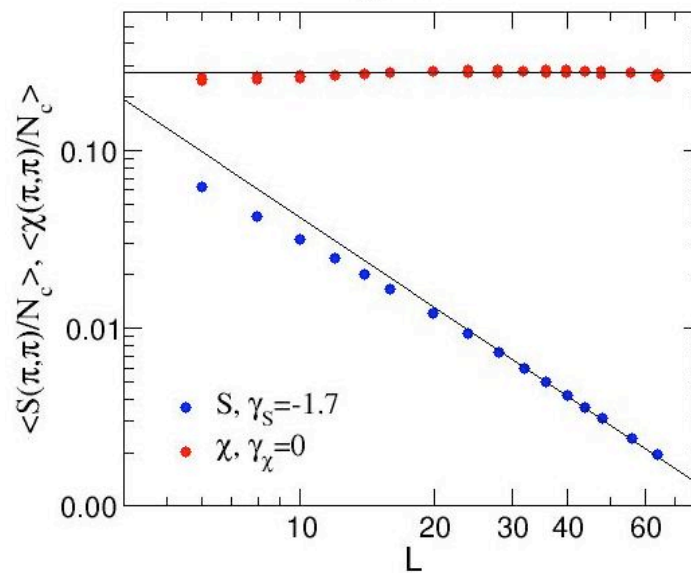
# No long-range order



Line of critical points  
with continuously  
varying exponents



$g=1.25$



$$S(\pi, \pi), \chi(\pi, \pi)$$

Finite-size scaling at  $g^*$

$$Z \approx 1.7$$

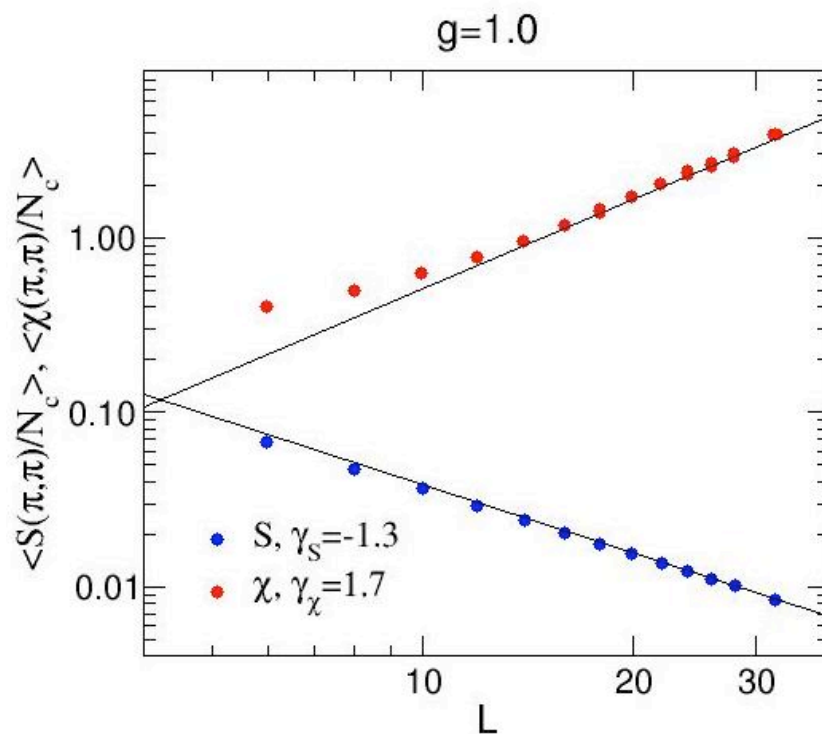
$S(\pi, \pi), \chi(\pi, \pi)$  Finite-size scaling at  $g=1.0$

$Z \approx 3.0$

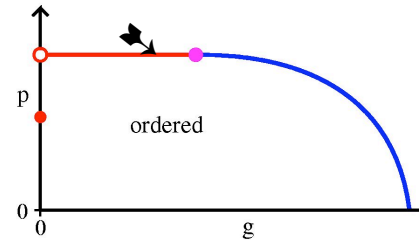
Disagrees with  $Z \approx 4.0$  from uniform susceptibility

None-asymptotic behavior?

Or problems related to disorder averaging?

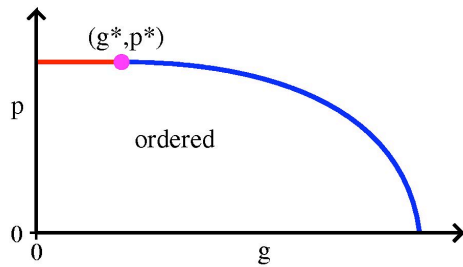


$z$  from  $\frac{\langle S \rangle}{\langle \chi \rangle}$  or  $\left\langle \frac{S}{\chi} \right\rangle$  ?

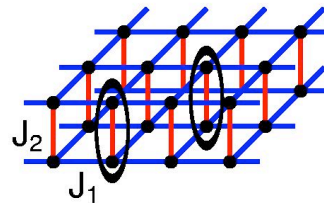


# Conclusions

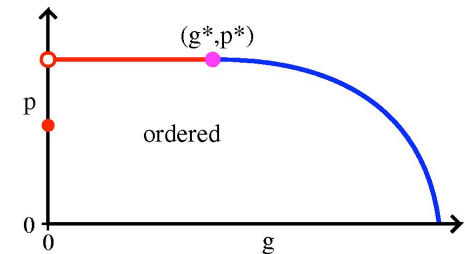
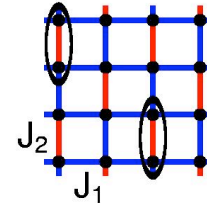
Novel quantum-critical behavior discovered numerically in dimer-diluted systems



percolation transition ending  
in multi-critical point



$$g = J_2/J_1$$



Line of critical points at  $p^*$

Conventional scaling for the  $p < p^*$  transition;  $z \approx 1.31$

Why does the single layer have a line of critical points?

Conditions under which the percolating cluster orders?