

## Deconfined quantum criticality

[Senthil et al., Science 303, 1490 (2004)]

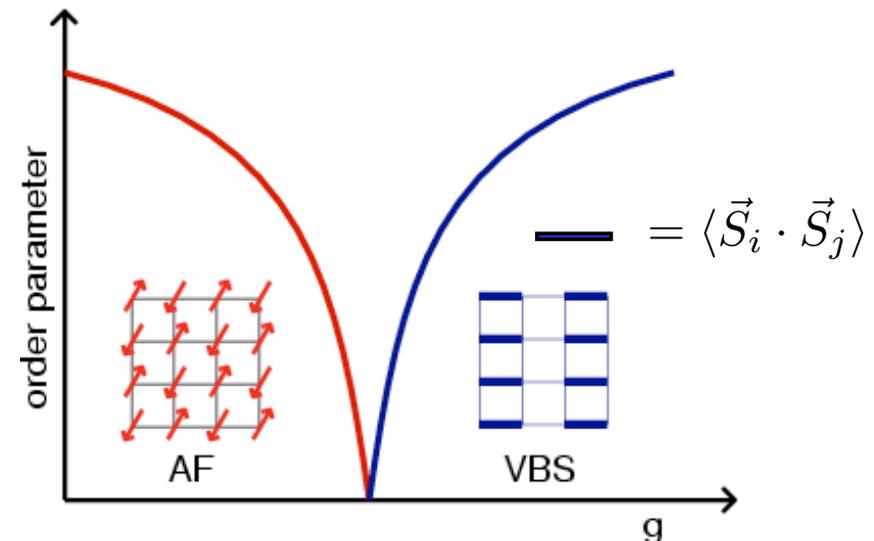
$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + g \times \dots$$

Quantum phase transition in a 2D system with one spin per unit cell

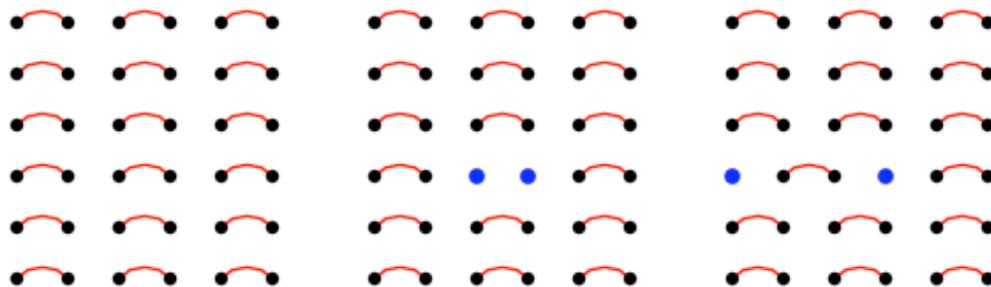
- antiferromagnetic for small  $g$
- valence-bond solid (VBS) for large  $g$  (spontaneously broken symmetry)

### Questions

- is the transition continuous?
  - ▶ normally order-order transitions are first order (Landau-Ginzburg)
  - ▶ theory of deconfined quantum critical points has continuous transition
- nature of the VBS fluctuations?
  - ▶ emergent U(1) symmetry predicted



### Spinon deconfinement upon approaching the critical point



Confinement inside VBS phase associated with new length scale and emergent U(1) symmetry

## How can we study deconfined quantum-criticality in a model system?

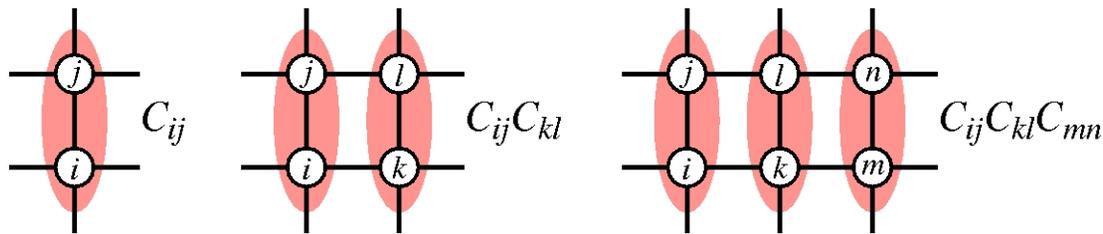
- the theory is based on continuum field-theory (Lagrangian)
- is there a reasonably microscopic model (Hamiltonian) with this physics?
- frustrated models (e.g.,  $J_1$ - $J_2$  Heisenberg) are good candidates
  - ▶ but no large-scale simulations (QMC) are possible
- **Look for non-frustrated models with Néel - VBS transition**

The Heisenberg interaction is equivalent to a singlet-projector

$$C_{ij} = \frac{1}{4} - \vec{S}_i \cdot \vec{S}_j$$

$$C_{ij}|\phi_{ij}^s\rangle = |\phi_{ij}^s\rangle, \quad C_{ij}|\phi_{ij}^{tm}\rangle = 0 \quad (m = -1, 0, 1)$$

- we can construct models with products of singlet projectors
- no frustration in the conventional sense (QMC can be used)
- multiple-singlet projection reduces the antiferromagnetic order



The original “J-Q” model is [Sandvik, PRL 2007]

$$H = -J \sum_{\langle ij \rangle} C_{ij} - Q \sum_{\langle ijkl \rangle} C_{ij} C_{kl}$$

- Has Néel-VBS transition, appears to be continuous (more later, with QMC)

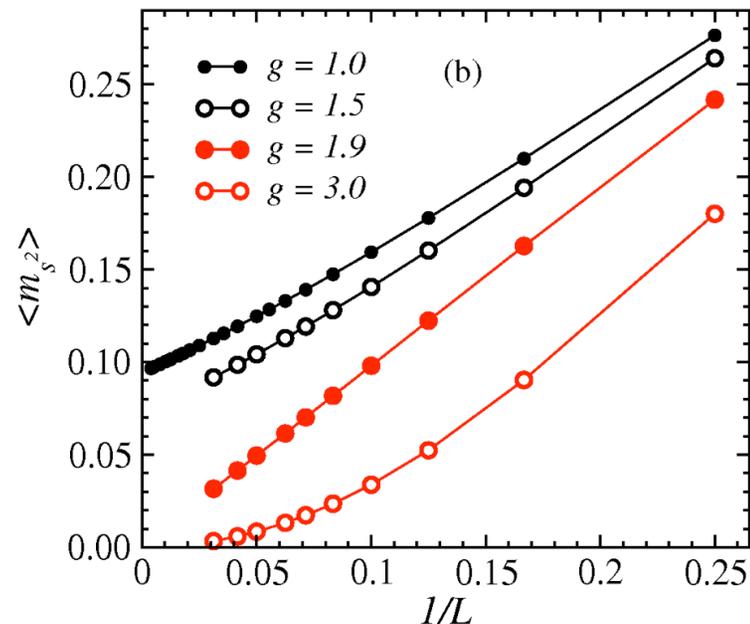
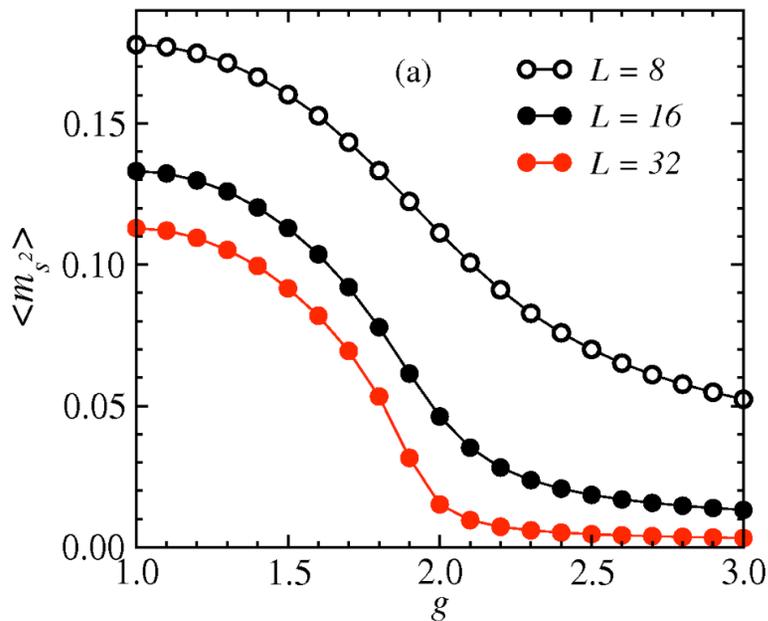
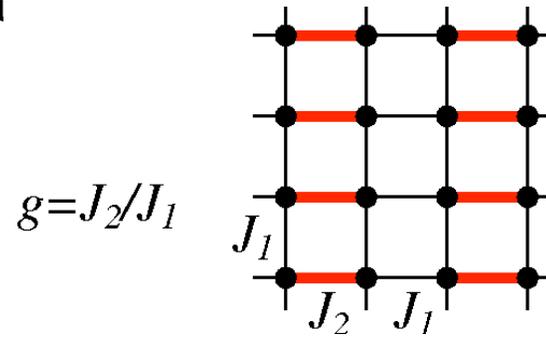
## Finite-lattice calculations

We will do numerically exact calculations (no approximations) for finite lattices

- extrapolate to infinite size, to learn about
  - ▶ the ground state and excitations
  - ▶ nature of quantum phase transitions
  - ▶ associated  $T > 0$  physics

**Example:** Dimerized Heisenberg model

- QMC results for  $L \times L$  lattices



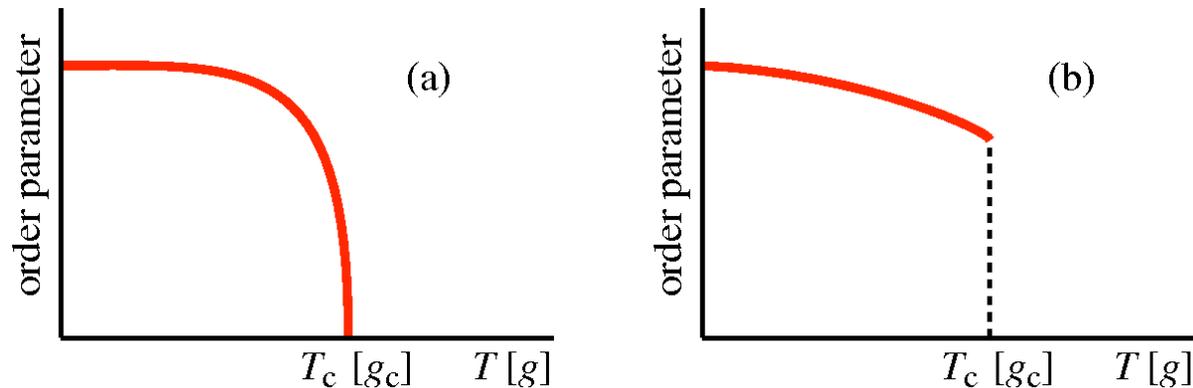
It is often known how various quantities should depend on  $L$

- in a Néel state, spin-wave theory  $\rightarrow \langle m_s^2(L) \rangle = \langle m_s^2(\infty) \rangle + a/L + \dots$
- use finite-size scaling theory to study the quantum-critical point

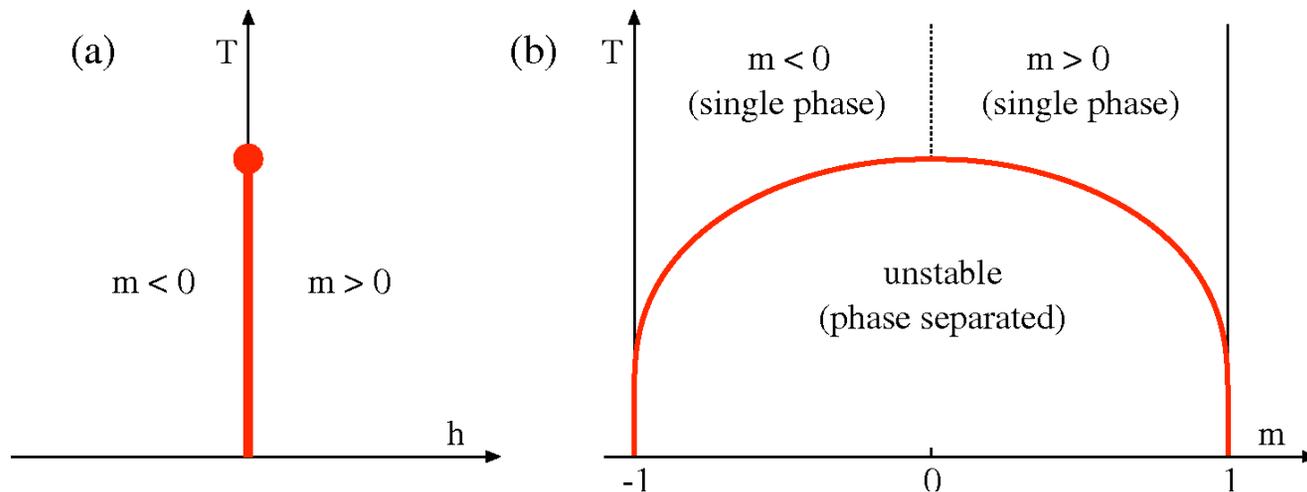
## Finite-size scaling and critical points

Phase transitions can be continuous or first-order (discontinuous)

- occur as a function of  $T$  or some parameter  $g$  at  $T=0$
- we want to analyze, especially, continuous transitions



Prototypical classical model with a critical point: 2D Ising model

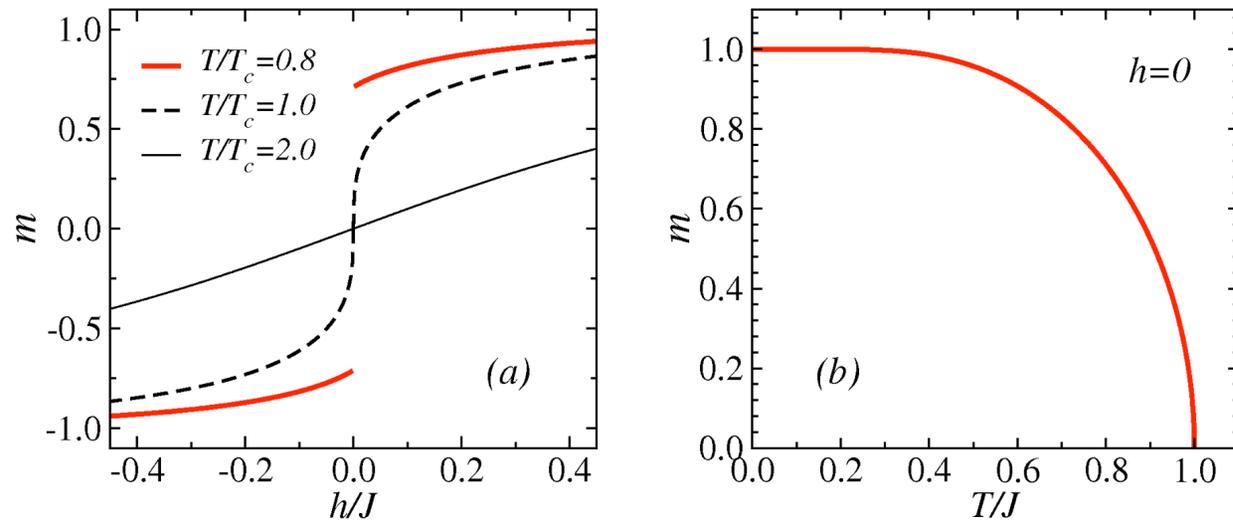


$$\frac{T_c}{J} = \frac{2}{\ln(1 + \sqrt{2})}$$

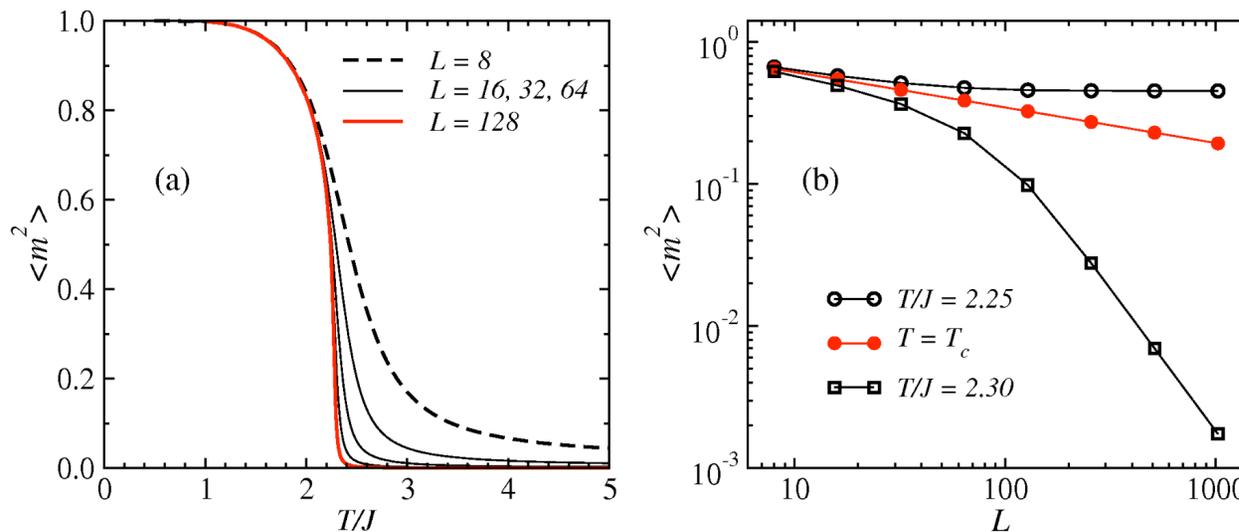
$$\approx 2.269$$

- first-order transition versus  $h$  (at  $h=0$ ) for  $T < T_c$
- continuous transition at  $h=0$

Mean-field solution:  $J = J_i = \sum_j J_{ij}$   $m = \tanh[(Jm + h)/T]$ ,  $(m = \langle \sigma_i \rangle)$



Monte Carlo results for  $L \times L$  lattices (cluster algorithm, very small error bars)



Phase transition becomes apparent for large  $L$

Critical exponent  $\beta$  can be extracted from  $L$ -scaling at  $T_c$

$$\langle m(\infty, T) \rangle \sim |T - T_c|^\beta$$

$$\langle m^2(L, T_c) \rangle \sim L^{-2\beta/\nu}$$

## Review of criticality and scaling

We discuss Ising spins for simplicity (but most results generic)

**Correlation function:**  $C(\mathbf{r}_{ij}) = \langle \sigma_i \sigma_j \rangle$

For large  $r$ :

$$C(r) \rightarrow \begin{cases} e^{-r/\xi} & T > T_c \\ r^{-(d-2+\eta)} & T = T_c \\ \langle m^2 \rangle & T < T_c \end{cases}$$

“Connected” correlation function for  $T < T_c$ :

$$\bar{C}(r) = C(r) - \langle |m| \rangle^2 \rightarrow e^{-r/\xi}$$

Note that the magnetization can be computed in a finite system in several ways, all equal when  $N \rightarrow \infty$ :

$$\langle |m| \rangle, \quad \sqrt{\langle m^2 \rangle}, \quad \sqrt{C(r_{\max})}, \quad \left[ m = \frac{1}{N} \sum_{i=1}^N \sigma_i \right]$$

The squared magnetization can be exactly written in terms of  $C(r)$ :

$$\langle m^2 \rangle = \frac{1}{N} \sum_{\mathbf{r}} C(\mathbf{r})$$

For  $N \rightarrow \infty$  close to  $T_c$ ,  $T < T_c$ :

$$\langle m \rangle \sim |t|^\beta, \quad t = (T - T_c)/T_c \quad \beta = \begin{cases} 1/8, & \text{2D Ising (exact)} \\ 1/2, & \text{mean - field (generic)} \\ \dots, & \text{other universality classes} \end{cases}$$

The correlation length diverges as  $T \rightarrow T_c$  (from above and below)

$$\xi \sim |t|^{-\nu}$$

2D Ising:  $\nu=1$ , mean-field:  $\nu=1/2, \dots$

Susceptibility (linear response function)

$$\chi = \left. \frac{d\langle m \rangle}{dh} \right|_{h \rightarrow 0} = \frac{N}{T} (\langle m^2 \rangle - \langle |m| \rangle^2)$$

also diverges as  $T \rightarrow T_c$

$$\chi \sim |t|^{-\gamma}$$

### **Finite-size scaling**

How are divergencies (and other singularities) affected by finite  $N$ ?

Consider some quantity which has the form ( $N=\infty$ )

$$Q \sim |t|^{-\kappa}$$

We can write  $|t|$  as:  $|t| \sim \xi^{-1/\nu}$ , which gives

$$Q \sim \xi^{\kappa/\nu}$$

The maximum correlation length is  $L$ , at  $T_c(L)$ . Substitute  $\xi \rightarrow L$

$$Q[T_c(L)] \sim L^{\kappa/\nu} \quad |t|_L = [T_c(L) - T_c(\infty)]/T_c(\infty) \sim L^{-1/\nu}$$

## More general finite-size scaling hypothesis

- has been justified using the renormalization-group theory

$$Q(t, L) = L^\sigma f(\xi/L),$$

Using  $\xi \sim |t|^{-1/\nu} \rightarrow$

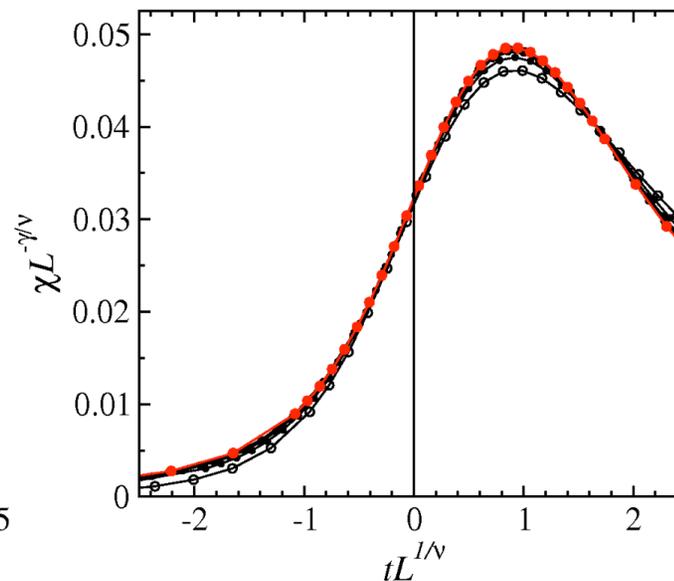
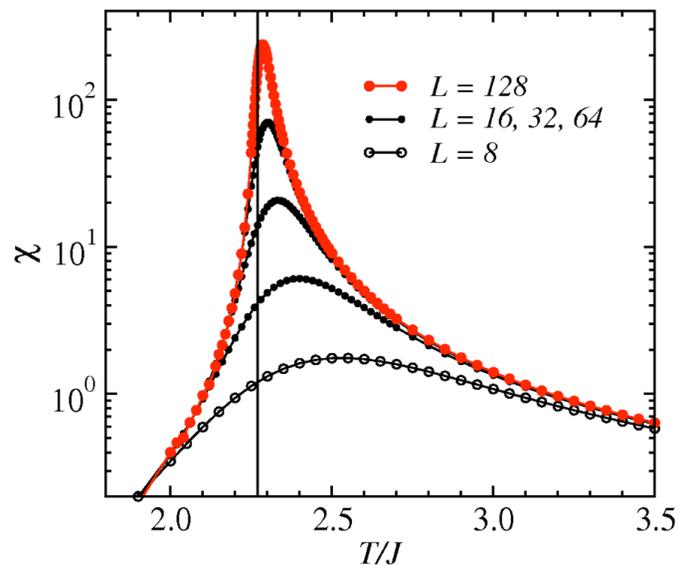
$$Q(t, L) = L^\sigma g(tL^{1/\nu})$$

From this we must be able to reproduce infinite-size form:

$$Q(t, L \rightarrow \infty) \sim |t|^{-\kappa}$$

which is the case if  $g(x) \sim x^{-\kappa}$  and  $\sigma = \kappa/\nu$

## Test: susceptibility of 2D Ising model (Monte Carlo)



$$T_c = 2/\ln(1 + \sqrt{2})$$

$$\nu = 1, \gamma = 7/4$$

Normally:  
adjust  $T_c$  and  
exponents so  
that the data  
“collapse”