

---

# Quantum phase transitions on percolating lattices

---

**Thomas Vojta**

Department of Physics, University of Missouri-Rolla



- Geometric percolation
  - Classical magnet on a percolating lattice
    - Percolation quantum phase transitions
- Quantum Ising magnet and activated scaling
  - Percolation and dissipation

---

# Acknowledgements

---

## currently at UMR

**Jose Hoyos**

Chetan Kotabage  
Man Young Lee

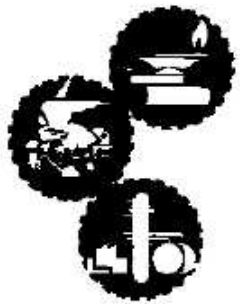
Shellie Huether  
Ryan Kinney  
Brett Sweeney

## former group members

Mark Dickison (Boston U.)  
Bernard Fendler (Florida State U.)  
Rastko Sknepnek (Iowa State U.)

## external collaboration

Ribhu Kaul (Duke U.)  
**Jörg Schmalian (Iowa State U.)**  
Matthias Vojta (U. of Cologne)



## Funding:

National Science Foundation  
Research Corporation  
University of Missouri Research Board



# Geometric percolation

- regular (square or cubic) lattice
- sites are occupied at random
  - site **empty** (vacancy) with probability  $p$
  - site **occupied** with probability  $1 - p$

**Question: Do the occupied sites form a connected infinite spanning cluster?**

- sharp **percolation threshold** at  $p_c$

$p > p_c$ : only disconnected finite-size clusters  
length scale: connectedness length  $\xi_c$

$p = p_c$ :  $\xi_c$  diverges, clusters on all scales, clusters are **fractals** with dimension  $D_f < d$

$p < p_c$ : infinite cluster covers finite fraction  $P_\infty$  of sites

$p > p_c$



$p = p_c$



$p < p_c$



# Percolation as a critical phenomenon

- percolation can be understood as continuous phase transition
- **geometric fluctuations** take the role of usual thermal or quantum fluctuations
- concepts of **scaling** and **critical exponents** apply

## cluster size distribution:

(number of clusters with  $s$  sites):

$$n_s(p) = s^{-\tau_c} f[(p - p_c) s^{\sigma_c}]$$

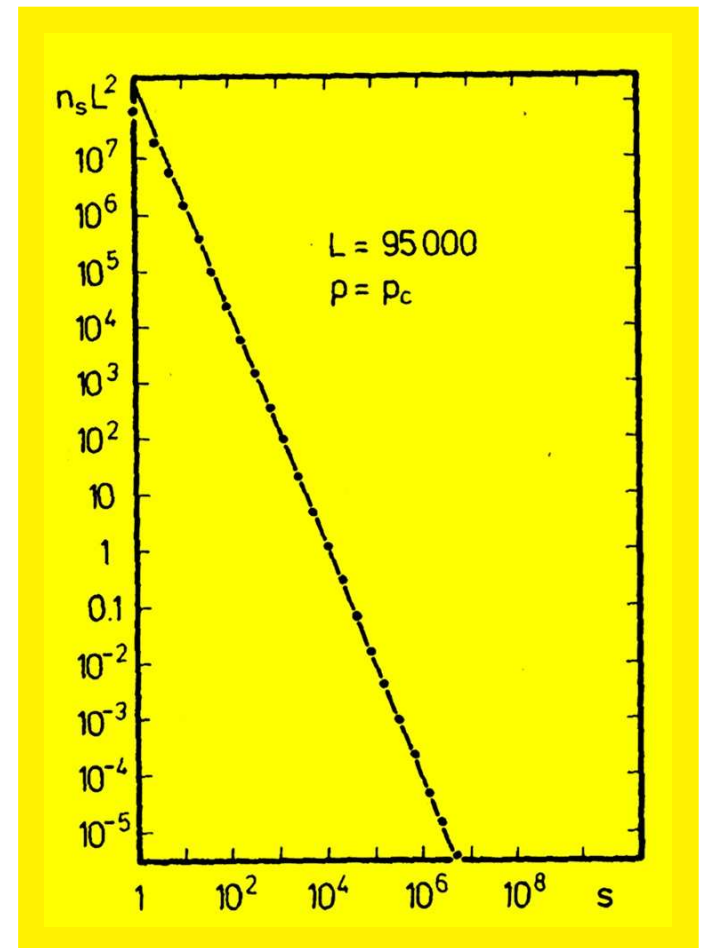
scaling function  $f(x)$

$$\begin{aligned} f(x) &\sim \exp(-B_1 x^{1/\sigma_c}) & (p > p_c) \\ f(x) &= \text{const} & (p = p_c) \\ f(x) &\sim \exp[-(B_2 x^{1/\sigma_c})^{1-1/d}] & (p < p_c) \end{aligned} .$$

**infinite cluster:**  $P_\infty \sim |p - p_c|^{\beta_c}$  ( $\beta_c = (\tau_c - 2)/\sigma_c$ )

**length scale :**  $\xi_c \sim |p - p_c|^{-\nu_c}$  ( $\nu_c = (\tau_c - 1)/d\sigma_c$ )

**fractal dimension:**  $D_f = d/(\tau_c - 1)$



from Stauffer/Aharony

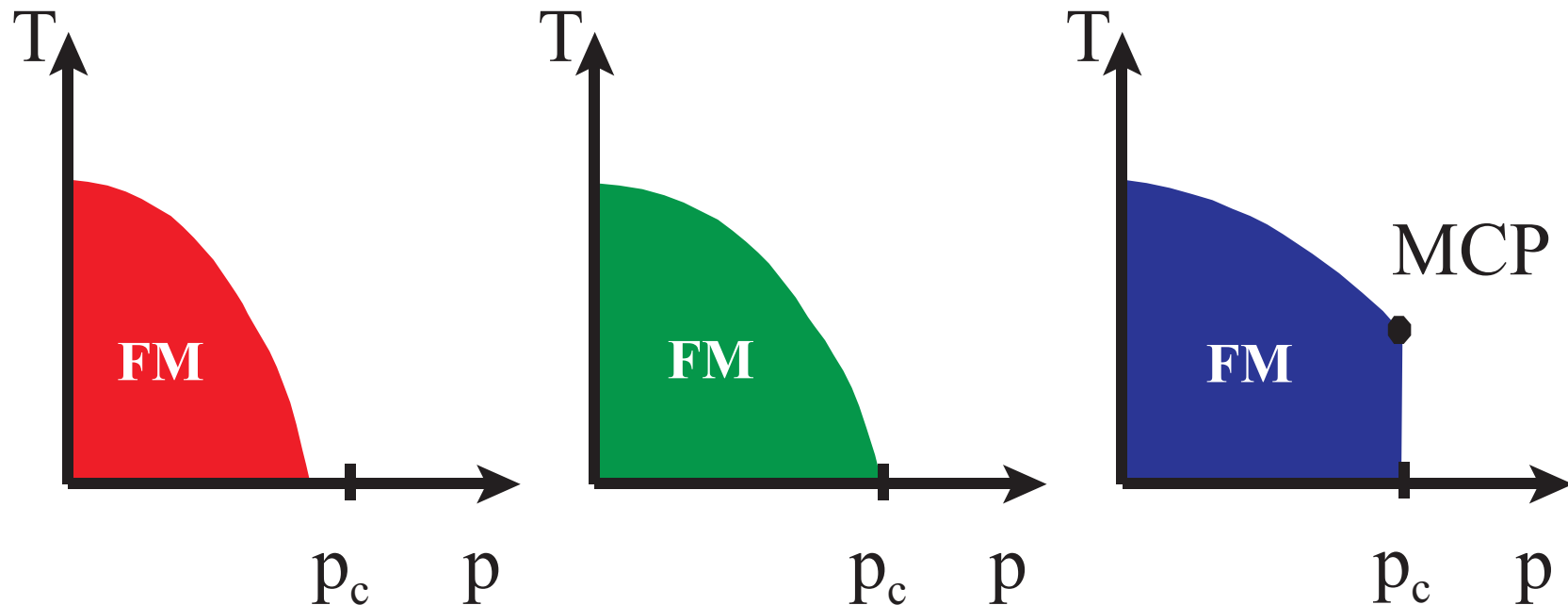
- 
- Geometric percolation
  - **Classical magnet on a percolating lattice**
    - Percolation quantum phase transitions
  - Quantum Ising magnet and activated scaling
    - Percolation and dissipation
-

## Classical diluted magnet

$$H = -J \sum_{\langle i,j \rangle} \epsilon_i \epsilon_j S_i S_j - h \sum_i \epsilon_i S_i$$

- $S_i$  – classical Ising or Heisenberg spin
- $\epsilon_i$  random variable, 0 with probability  $p$ , 1 with probability  $1 - p$

**Question:**  
Phase diagram as function of temperature  $T$   
and impurity concentration  $p$ ?



---

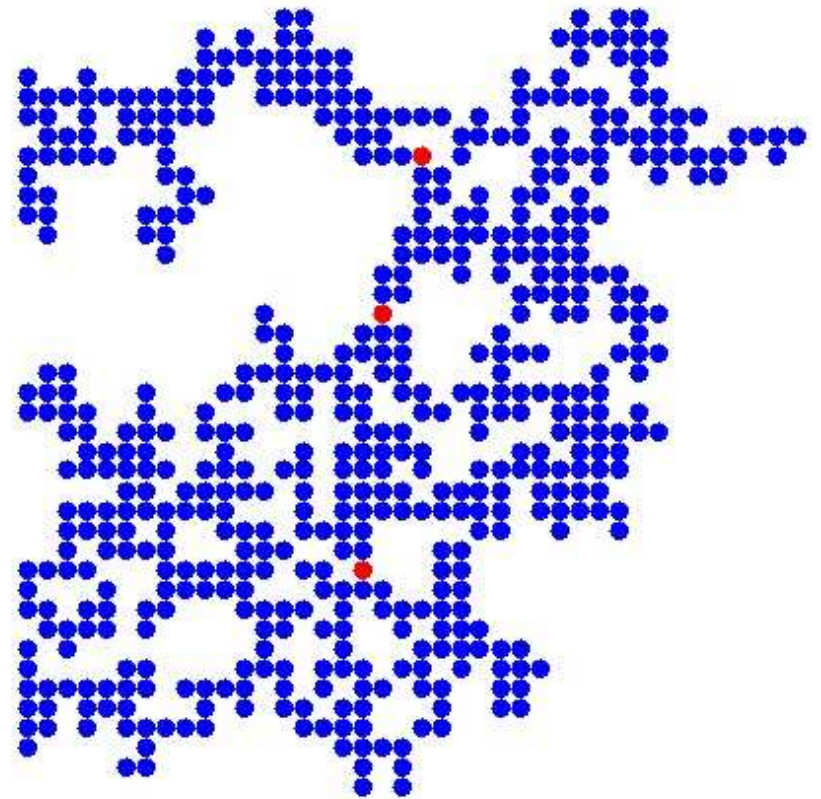
# Is a classical magnet on the critical percolation cluster ordered?

---

**naive argument:** fractal dimension  $D_f > 1 \Rightarrow$  Ising magnet orders at low  $T$

**Wrong !!!**

- critical percolation cluster contains **red sites**
  - parts on both sides of red site can be flipped with **finite energy cost**
- $\Rightarrow$  no long-range order at any finite  $T$ ,  
 $T_c(p)$  **vanishes at percolation threshold**
- fractal (mass) dimension  $D_f$  not sufficient to characterize magnetic order



- 
- Geometric percolation
    - Classical magnet on a percolating lattice
    - **Percolation quantum phase transitions**
  - Quantum Ising magnet and activated scaling
    - Percolation and dissipation



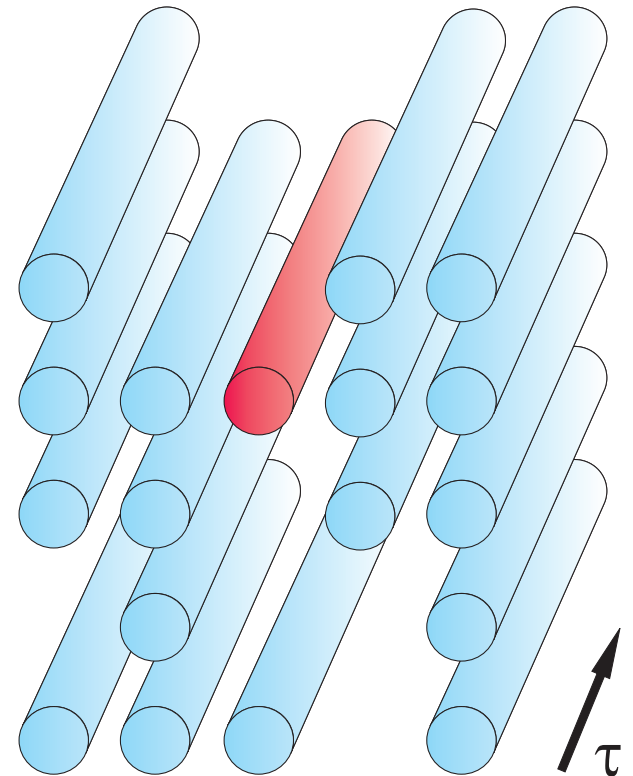
# Percolation and quantum fluctuations

- quantum fluctuations are less effective in destroying long-range order
- red sites  $\Rightarrow$  **red lines, infinite at  $T = 0$**
- flipping cluster parts on both sides of red line requires **infinite energy**

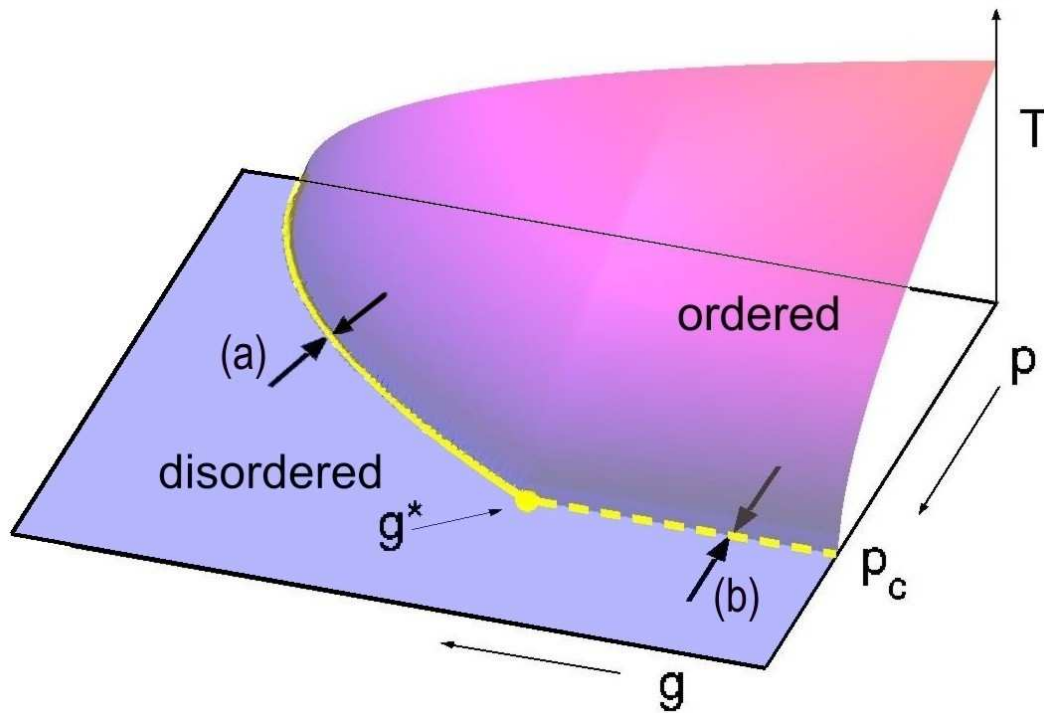
**Long-range order survives on the critical percolation cluster**

(if quantum fluctuations are not too strong)

(confirmed by explicit results for quantum Ising and Heisenberg magnets and for quantum rotors)



# Phase diagram of a diluted quantum magnet



## Schematic phase diagram

$p$  = impurity concentration

$g$  = quantum fluctuation strength

$T$  = temperature

(long-range order at  $T > 0$  requires  $d \geq 2$  for Ising and  $d \geq 3$  for Heisenberg symmetry)

## Two zero-temperature quantum phase transitions:

(a) generic quantum phase transition, driven by **quantum fluctuations**

(b) percolation quantum phase transition, driven by **geometry of the lattice**

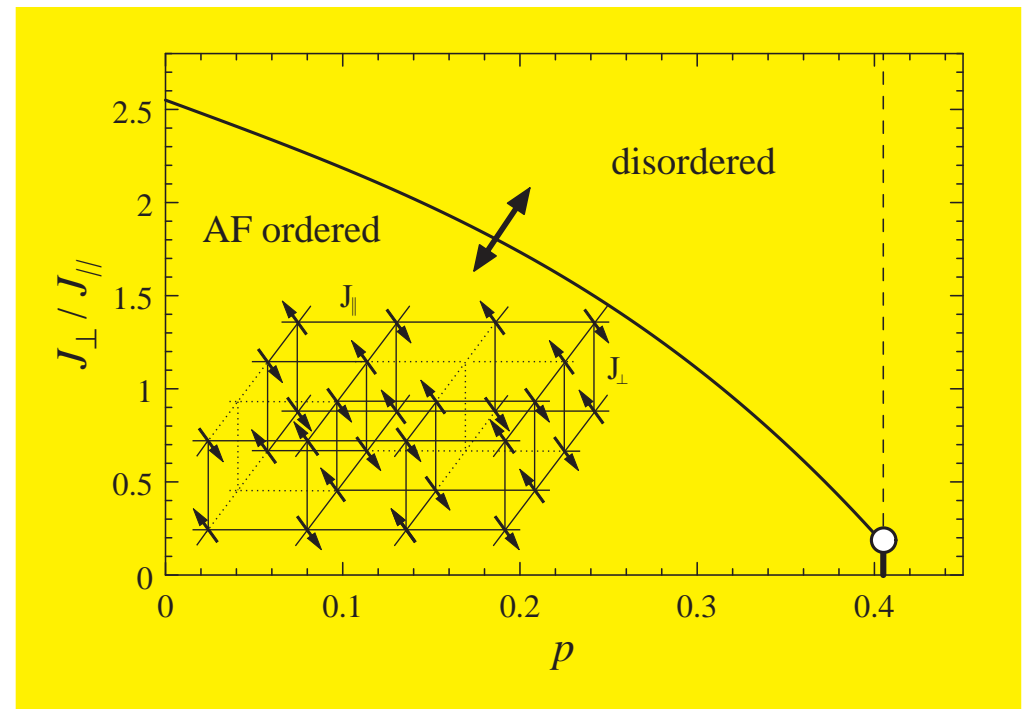
transitions separated by **multicritical point** at  $(g^*, p_c, T = 0)$

# Example: diluted bilayer Heisenberg antiferromagnet

$$H = J_{\parallel} \sum_{\substack{\langle i,j \rangle \\ a=1,2}} \epsilon_i \epsilon_j \hat{\mathbf{S}}_{i,a} \cdot \hat{\mathbf{S}}_{j,a} + J_{\perp} \sum_i \epsilon_i \hat{\mathbf{S}}_{i,1} \cdot \hat{\mathbf{S}}_{i,2},$$

- $\hat{\mathbf{S}}_{j,a}$ : quantum spin operator ( $S = 1/2$ ) at site  $j$ , layer  $a$
- ratio  $J_{\perp}/J_{\parallel}$  controls strength of **quantum** fluctuations
- **dilution**: random variable  $\epsilon_i=0,1$  with probabilities  $p, 1 - p$ .

Phase diagram mapped out by Sandvik (2002) and Vajk and Greven (2002)



---

# Model action, order parameter, and correlation length

---

## $O(N)$ quantum rotor model ( $N \geq 2$ )

$$\mathcal{A} = \int d\tau \sum_{\langle ij \rangle} J \epsilon_i \epsilon_j \mathbf{S}_i(\tau) \cdot \mathbf{S}_j(\tau) + \frac{T}{g} \sum_i \sum_n \epsilon_i |\omega_n|^{2/z_0} \mathbf{S}_i(\omega_n) \mathbf{S}_i(-\omega_n)$$

$\mathbf{S}_i(\tau)$ :  $N$ -component unit vector at site  $i$  and imaginary time  $\tau$

$\epsilon_i = 0, 1$ : random variable describing site dilution

$z_0$ : (bare) dynamical exponent of the clean system.

### Order parameter (magnetization):

- magnetic long-range order only possible on infinite percolation cluster
- for  $g < g^*$ , infinite percolation cluster is ordered for all  $p < p_c$

$\Rightarrow$  magnetization  $m \sim P_\infty \sim |p - p_c|^{\beta_c}$

$$\beta = \beta_c$$

### Spatial correlation length:

- magnetic correlations cannot extend beyond connectedness length of the lattice

$\Rightarrow$  correlation length  $\xi \sim \xi_c \sim |p - p_c|^{-\nu_c}$

$$\nu = \nu_c$$

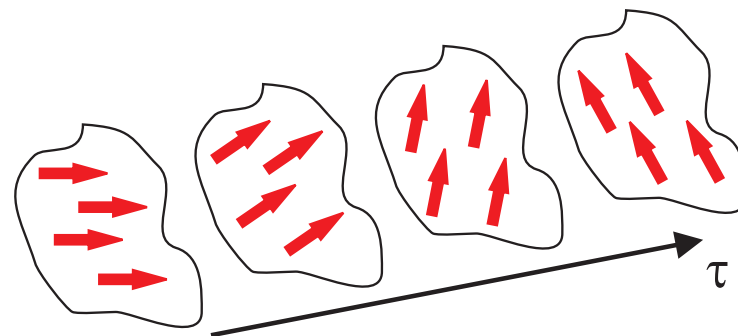
---

# Quantum dynamics of a single percolation cluster

---

## single percolation cluster of $s$ sites

- for  $g < g^*$ , all rotors on the cluster are correlated but collectively fluctuate in time
- ⇒ cluster acts as single (0+1) dimensional NLSM model with moment  $s$



$$\mathcal{A}_s = s \frac{T}{g} \sum_i \sum_n |\omega_n|^{2/z_0} \mathbf{S}(\omega_n) \mathbf{S}(-\omega_n) + sh \int d\tau S^{(1)}(\tau)$$

## Dimensional analysis or renormalization group calculation:

$$F_s(g, h, T) = g^\varphi s^{-\varphi} \Phi(h s^{1+\varphi} g^{-\varphi}, T s^\varphi g^{-\varphi}) \quad \varphi = z_0 / (2 - z_0)$$

- free energy of quantum spin cluster **more singular** than that of classical spin cluster
- **susceptibility**: classically  $\chi_s^c \sim s^2$ , quantum (at  $T = 0$ ):  $\chi_s \sim s^{2+\varphi}$   
susceptibility of quantum cluster diverges faster with cluster size  $s$

---

# Scaling theory of the percolation quantum phase transition

---

- total free energy is sum over contributions of all percolation clusters
- combining **percolation cluster size distribution** + **free energy of single cluster**

$$F(p - p_c, h, T) = \sum_s n_s(p - p_c) F_s(g, h, T)$$

## Scaling form of free energy:

- rescaling  $s \rightarrow s/b^{D_f}$  yields

$$F(p - p_c, h, T) = b^{-(d+z)} F\left((p - p_c)b^{1/\nu}, hb^{(D_f+z)}, Tb^z\right)$$

- correlation length exponent identical to the classical value,  $\nu = \nu_c$
- $z = \varphi D_f$  plays the role of the dynamic critical exponent.

# Critical behavior

- exponents determined by two lattice percolation exponents (e.g.,  $\nu = \nu_c$ ,  $D_f$ ) and the **dynamical exponent**  $z$

$$2 - \alpha = (d + z) \nu$$

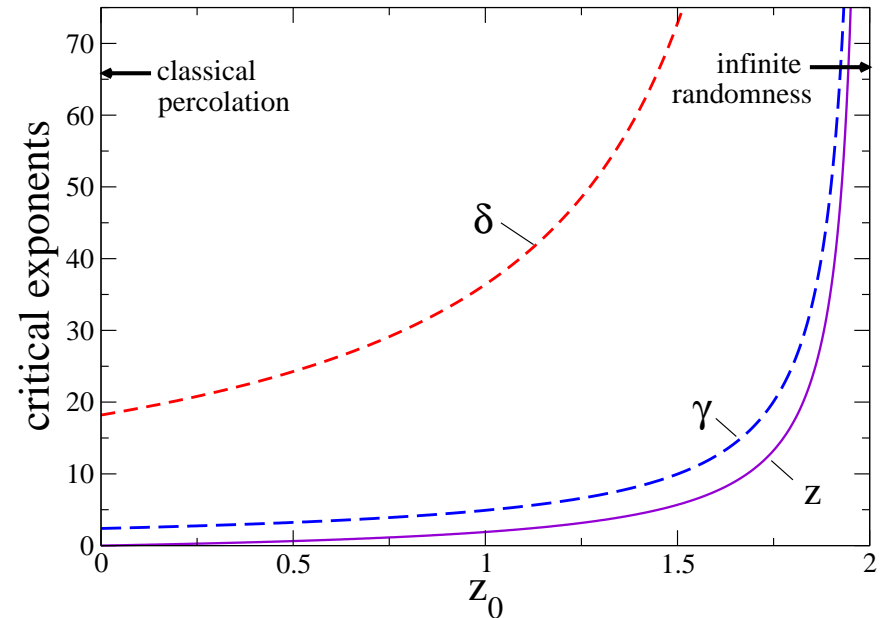
$$\beta = (d - D_f) \nu$$

$$\gamma = (2D_f - d + z) \nu$$

$$\delta = (D_f + z) / (d - D_f)$$

$$2 - \eta = 2D_f - d + z .$$

- classical** exponents recovered for  $z = 0$ :
- $\alpha$ ,  $\gamma$ ,  $\delta$ , and  $\eta$  are **nonclassical** while  $\beta$  is **unchanged**



Exponents in 2D as function of  $z_0$ .

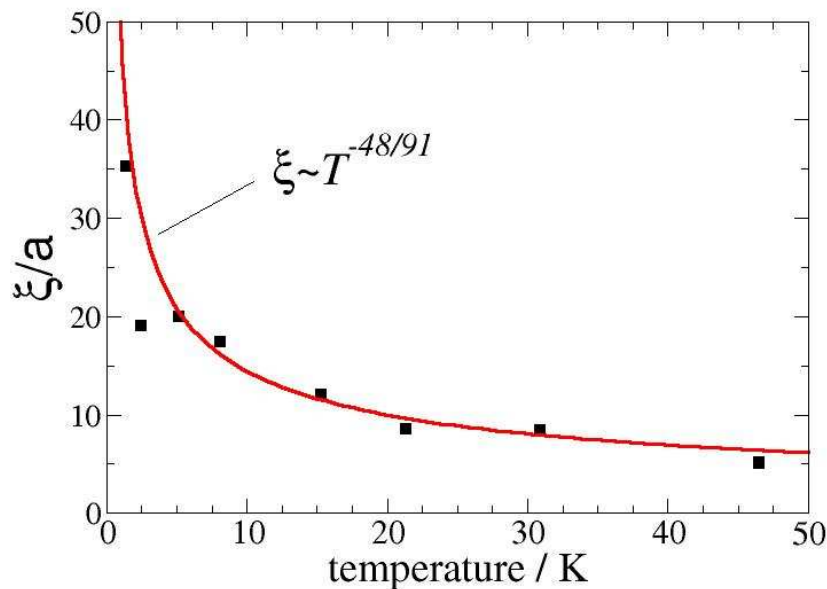
	2d		3d	
	classical	quantum	classical	quantum
$\alpha$	$-2/3$	$-115/36$	$-0.62$	$-2.83$
$\beta$	$5/36$	$5/36$	$0.417$	$0.417$
$\gamma$	$43/18$	$59/12$	$1.79$	$4.02$
$\delta$	$91/5$	$182/5$	$5.38$	$10.76$
$\nu$	$4/3$	$4/3$	$0.875$	$0.875$
$\eta$	$5/24$	$-27/16$	$-0.06$	$-2.59$
$z$	-	$91/48$	-	$2.53$

Exponents in 2d and 3d for  $z_0 = 1$ .

# Simulation and experiment

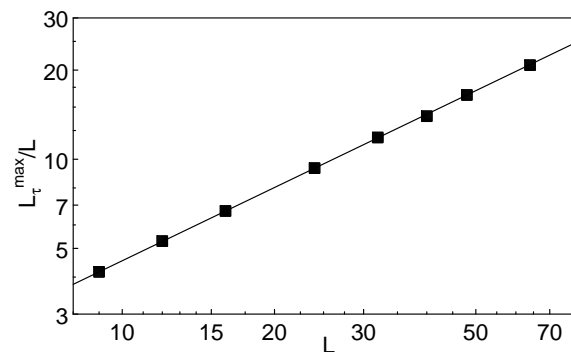
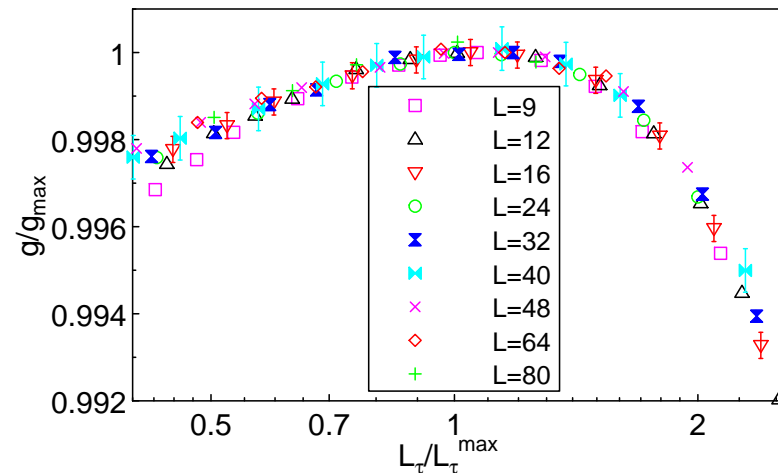
## Diluted Heisenberg antiferromagnet $\text{La}_2\text{Cu}_{1-x}(\text{Zn,Mg})_x\text{O}_4$

- neutron scattering experiments  
Vajk et al., Science 295, 1691, (2002)
- correlation length at  $p = p_c$   
prediction  $\xi \sim T^{-1/z}$



## Monte-Carlo simulations

- FSS of Binder cumulant at  $p = p_c$   
 $\Rightarrow z \approx 1.83$



R. Sknepnek, M.V., T.V., PRL **93**, 097201 (2004),  
T.V., R. Sknepnek PRB **74**, 094415 (2006)



- 
- Geometric percolation
  - Classical magnet on a percolating lattice
    - Percolation quantum phase transitions
  - **Quantum Ising magnet and activated scaling**
    - Percolation and dissipation
-

---

## Diluted transverse-field Ising model

---

$$H_I = -J \sum_{\langle i,j \rangle} \epsilon_i \epsilon_j \hat{S}_i^z \hat{S}_j^z - h_x \sum_i \epsilon_i \hat{S}_i^x - h_z \sum_i \epsilon_i \hat{S}_i^z ,$$

- $\hat{S}_j^{x,z}$ :  $x$  and  $z$  components of quantum spin operator ( $S = 1/2$ ) at site  $j$
- $h_x$ : transverse magnetic field, controls strength of **quantum** fluctuations
- $h_z$ : ordering (longitudinal) magnetic field, conjugate to order parameter
- **dilution**: random variable  $\epsilon_i=0,1$  with probabilities  $p, 1 - p$ .

### single percolation cluster of $s$ sites

- for small  $h_x$ , all spins on the cluster are correlated but collectively fluctuate in time
- cluster of size  $s$  acts as (0+1) dimensional **Ising model** with moment  $s$
- energy gap (inverse susceptibility) of cluster depends **exponentially** on size  $s$

$$\Delta \sim \chi_s^{-1} \sim h_x e^{-Bs} \quad [B \sim \ln(J/h_x)]$$

---

## Activated scaling

---

- exponential relation between length and time scales:  $\ln \xi_\tau \sim \ln(1/\Delta) \sim s \sim \xi^{D_f}$

$$\text{Activated scaling: } \ln \xi_\tau \sim \xi^{D_f}$$

### Scaling form of the magnetization at the percolation transition

(Senthil/Sachdev 96)

- sum over all percolation clusters using size distribution  $n_s$

$$m(p - p_c, h_z) = b^{-\beta_c/\nu_c} m\left((p - p_c)b^{1/\nu_c}, \ln(h_z)b^{-D_f}\right)$$

- at the percolation threshold  $p = p_c$ :  $m \sim [\ln(h_z)]^{2-\tau_c}$
- for  $p \neq p_c$ : power-law quantum Griffiths effects  $m \sim h_z^\zeta$  with nonuniversal  $\zeta$

- 
- Geometric percolation
  - Classical magnet on a percolating lattice
    - Percolation quantum phase transitions
  - Quantum Ising magnet and activated scaling
    - **Percolation and dissipation**
-

---

# Dissipative transverse-field Ising model

---

- couple each spin to local bath of harmonic oscillators

$$H = H_I + \sum_{i,n} \epsilon_i \left[ \nu_{i,n} a_{i,n}^\dagger a_{i,n} + \frac{1}{2} \lambda_{i,n} \hat{S}_i^z (a_{i,n}^\dagger + a_{i,n}) \right]$$

- $a_{i,n}^\dagger, a_{i,n}$ : creation and destruction operator of the  $n$ -th oscillator coupled to spin  $i$
- $\nu_{i,n}$  frequency of of the  $n$ -th oscillator coupled to spin  $i$
- $\lambda_{i,n}$ : coupling constant

**Ohmic dissipation:** spectral function of the baths is **linear** in frequency

$$\mathcal{E}(\omega) = \pi \sum_n \lambda_{i,n}^2 \delta(\omega - \nu_{i,n}) / \nu_{i,n} = 2\pi \alpha \omega e^{-\omega/\omega_c}$$

$\alpha$  dimensionless dissipation strength

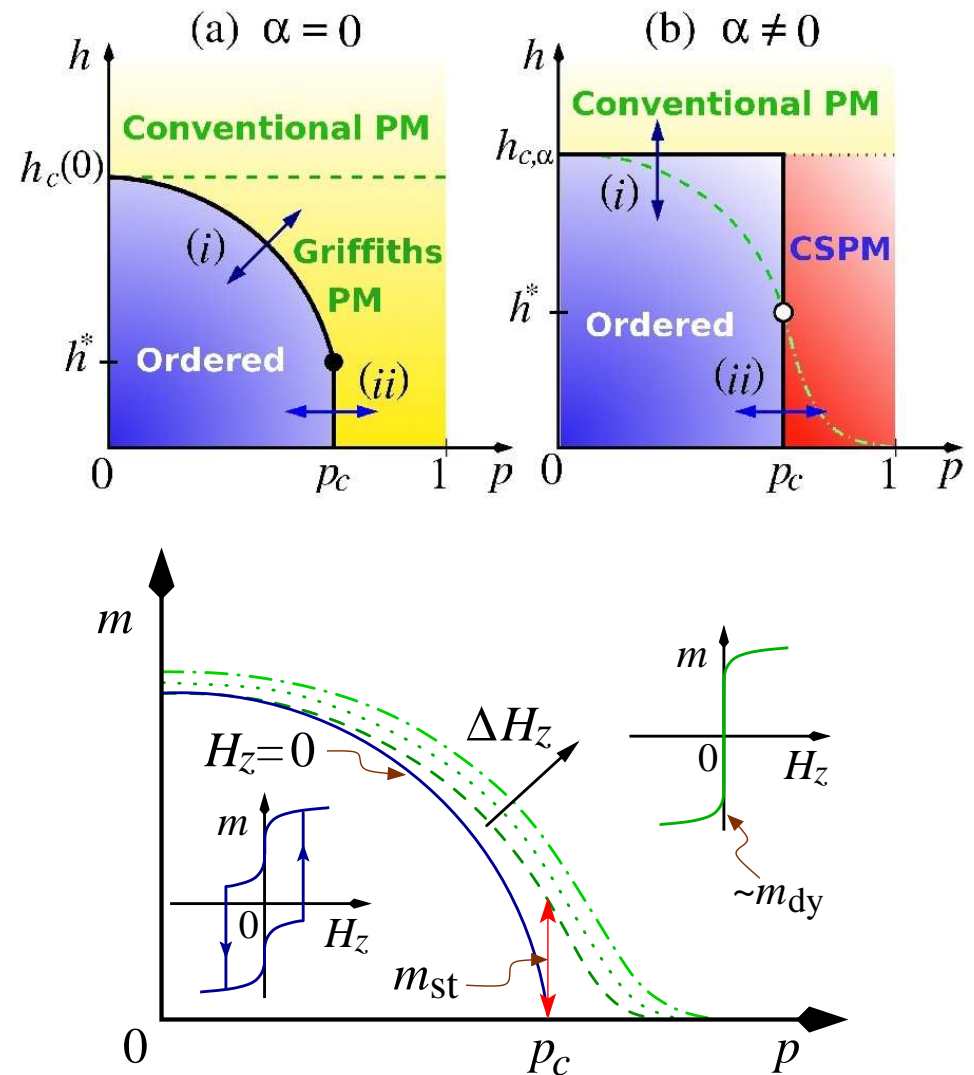
$\omega_c$  cutoff energy

# Phase diagram

- percolation cluster of size  $s$  equivalent to **dissipative** two-level system with effective dissipation strength  $s\alpha$
- $\Rightarrow$  **large clusters** with  $s\alpha > 1$  **freeze**  
**small clusters** with  $s\alpha < 1$  **fluctuate**
- frozen clusters act as classical superspins, dominate low-temperature susceptibility

$$\chi \sim |p - p_c|^{-\gamma_c}/T$$

- magnetization of infinite cluster  
 $m_\infty \sim P_\infty(p) \sim |p - p_c|^\beta$
- magnetization of finite-size frozen and fluctuating clusters leads to **unusual hysteresis effects**



---

## Conclusions

---

- long-range order on critical percolation cluster is destroyed by thermal fluctuations  
**long-range order survives a nonzero amount of quantum fluctuations**  
⇒ permits **percolation quantum phase transition**
- critical behavior is controlled by lattice percolation exponents but it is **different from classical percolation**
- in diluted quantum Ising magnets ⇒ exotic transition, activated scaling
- Ohmic dissipation: large percolation clusters **freeze**, act as **superspins**  
⇒ **classical superparamagnetic cluster phase**

**Interplay between geometric criticality and quantum fluctuations leads to novel quantum phase transition universality classes**