Quantum phase transitions on percolating lattices

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1. **Geometric percolation**
2. **Classical magnet on a percolating lattice**
3. **Quantum phase transitions and percolation**
   - Transverse-field Ising magnet
   - Bilayer quantum Heisenberg magnet
   - Percolation and dissipation

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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 ξ_c

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

$p < p_c$: infinite cluster covers finite fraction P_∞ 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

number of sites in infinite cluster: $P_\infty \sim |p - p_c|^{\beta_c}$

connectedness length: $\xi_c \sim |p - p_c|^{-\nu_c}$

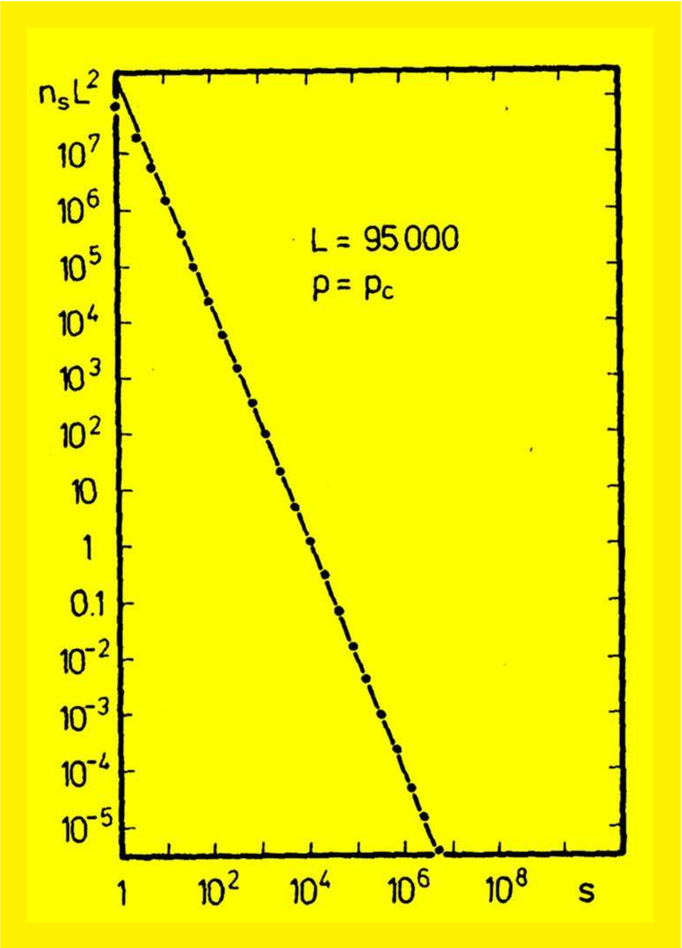
cluster size distribution:
(number of clusters with s sites):

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

scaling function $f(x)$

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

exponents are known exactly in 2D, numerically in 3D



from Stauffer/Aharony

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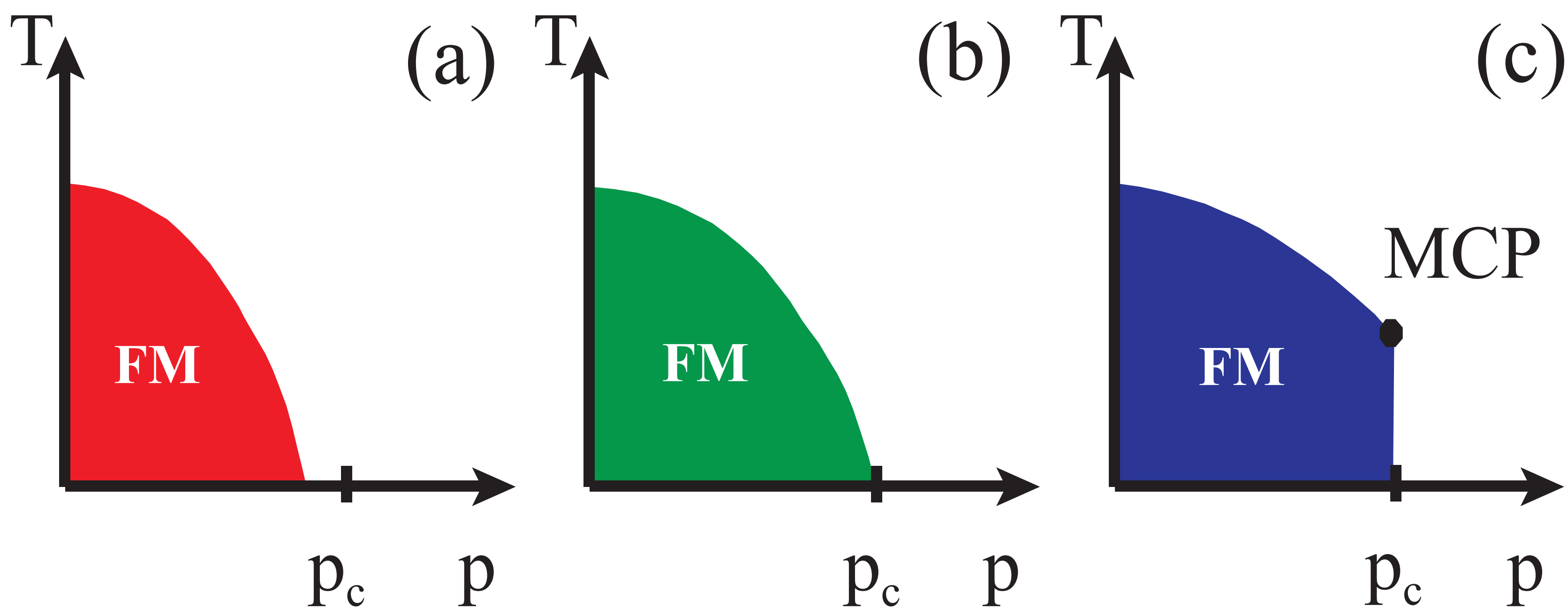
Classical diluted magnet

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

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

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

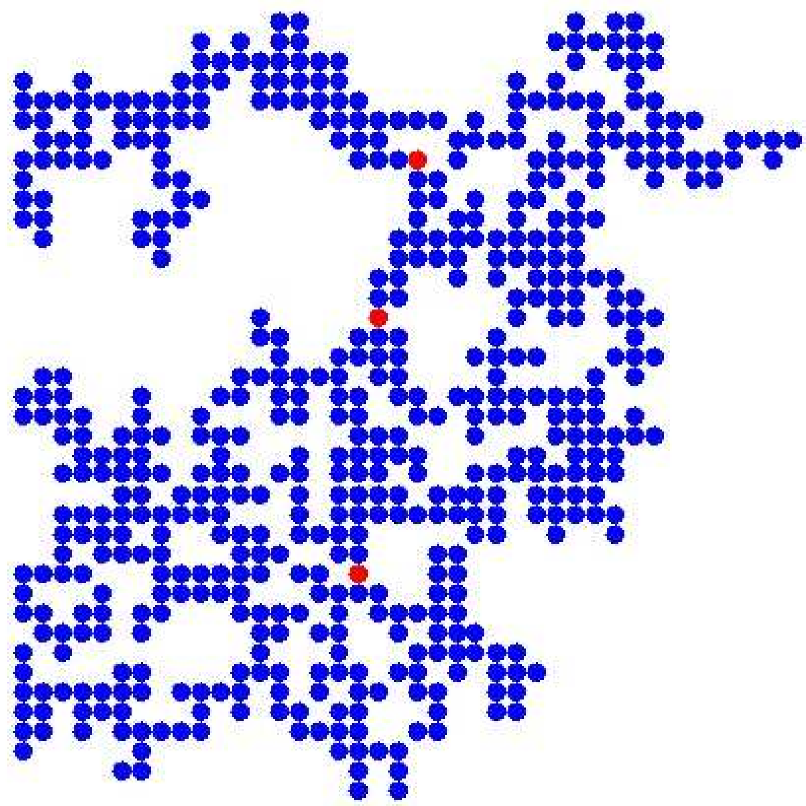


Is a classical magnet on the critical percolation cluster ordered?

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**
- fractal (mass) dimension D_f not sufficient to characterize magnetic order



$\Rightarrow$ no long-range order at any finite T,
$T_c(p)$ **vanishes at percolation threshold**

$\Rightarrow$ **phase diagram is of type (b)**

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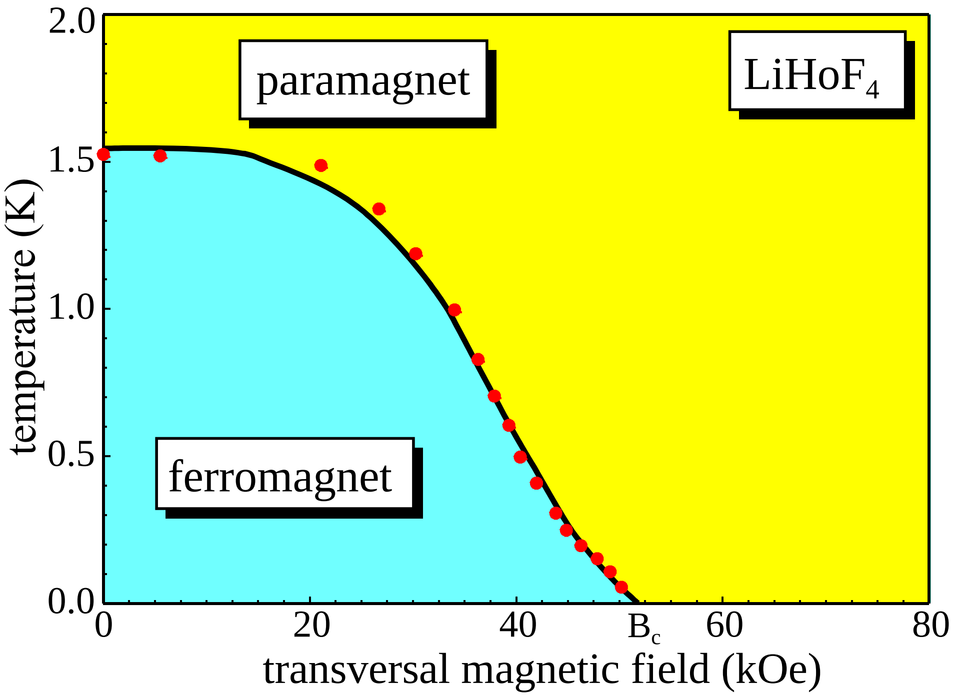
Quantum phase transitions

occur at **zero temperature** as function of pressure, magnetic field, chemical composition, ...

driven by **quantum** rather than thermal fluctuations



phase diagram of $LiHoF_4$ (Bitko et al. 96)

Transverse-field Ising model

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

transverse magnetic field induces spin flips via $\hat{S}^x = \hat{S}^+ + \hat{S}^-$

transverse field suppresses magnetic order

Imaginary time and quantum to classical mapping

Classical partition function: statics and dynamics decouple

$$Z = \int dpdq\ e^{-\beta H(p,q)} = \int dp\ e^{-\beta T(p)} \int dq\ e^{-\beta U(q)} \sim \int dq\ e^{-\beta U(q)}$$

Quantum partition function: statics and dynamics coupled

$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \lim_{N\to\infty} (e^{-\beta \hat{T}/N} e^{-\beta \hat{U}/N})^N = \int D[q(\tau)]\ e^{S[q(\tau)]}$$

imaginary time τ acts as additional dimension
at $T = 0$, the extension in this direction becomes infinite

Caveats:

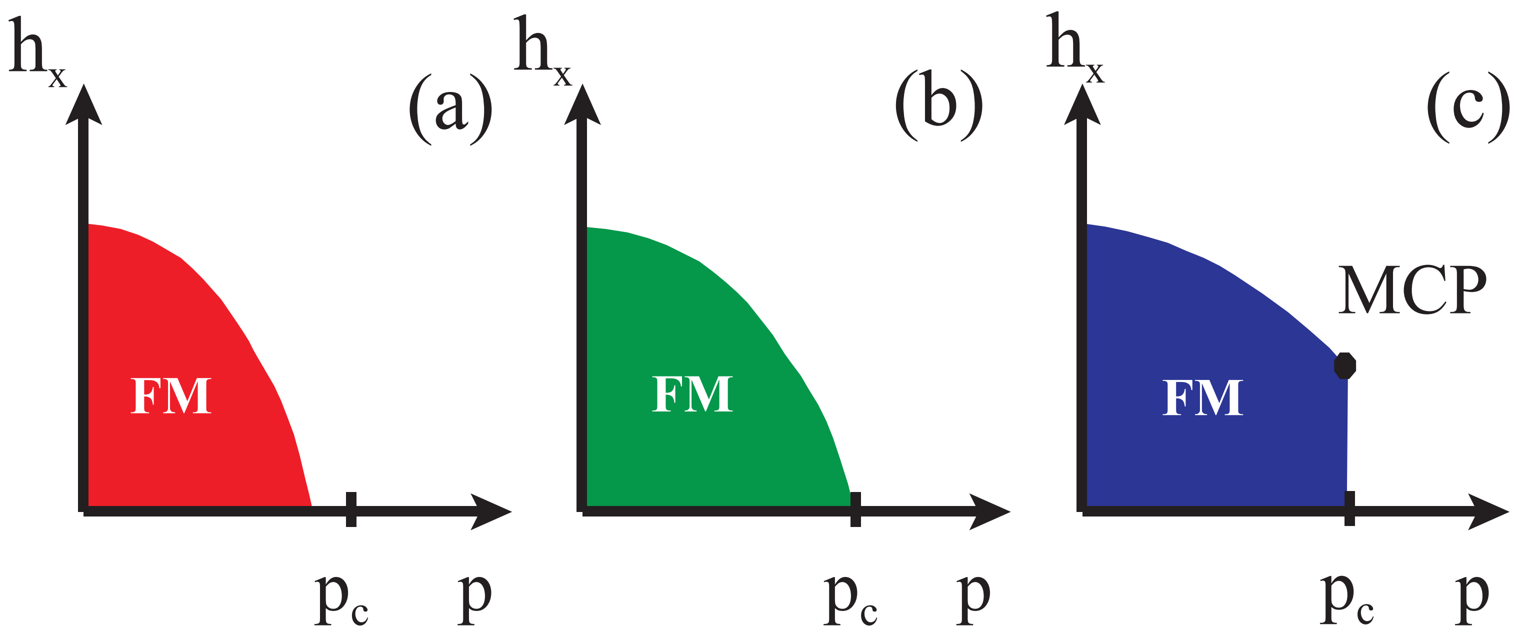
- mapping holds for thermodynamics only
- resulting classical system can be unusual and anisotropic ($z \neq 1$)
- extra complications with no classical counterpart may arise, e.g., Berry phases

Diluted transverse-field Ising model

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

- first term: interaction between the z-components of the spins
- second term: transverse magnetic field, controls quantum fluctuations
- third term: external magnetic field in z-direction, conjugate to order parameter

Zero-temperature phase diagram as function of transverse field h_x and impurity concentration p?



Red sites versus red lines

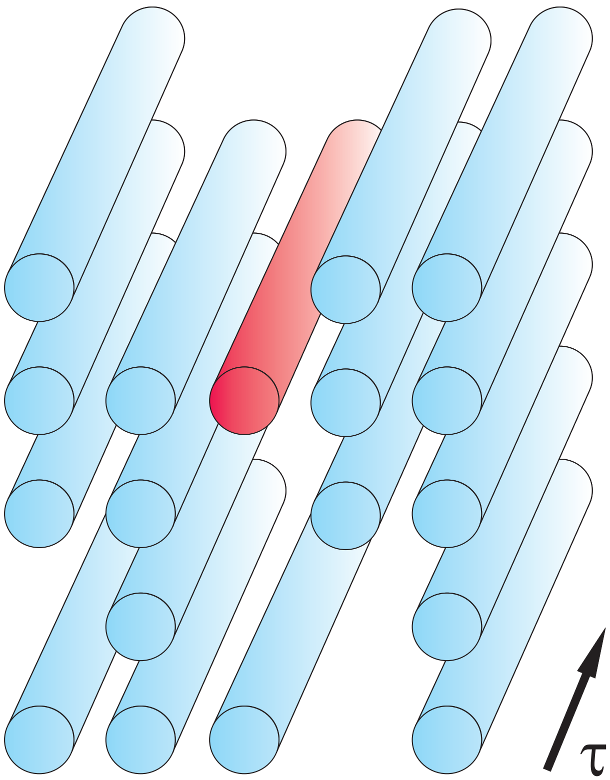
- quantum fluctuations are less effective in destroying long-range order
- red sites ⇒ **red lines, infinite at $T = 0$**
- flipping cluster parts on both sides of red line requires **infinite energy**

Long-range order survives on the critical percolation cluster

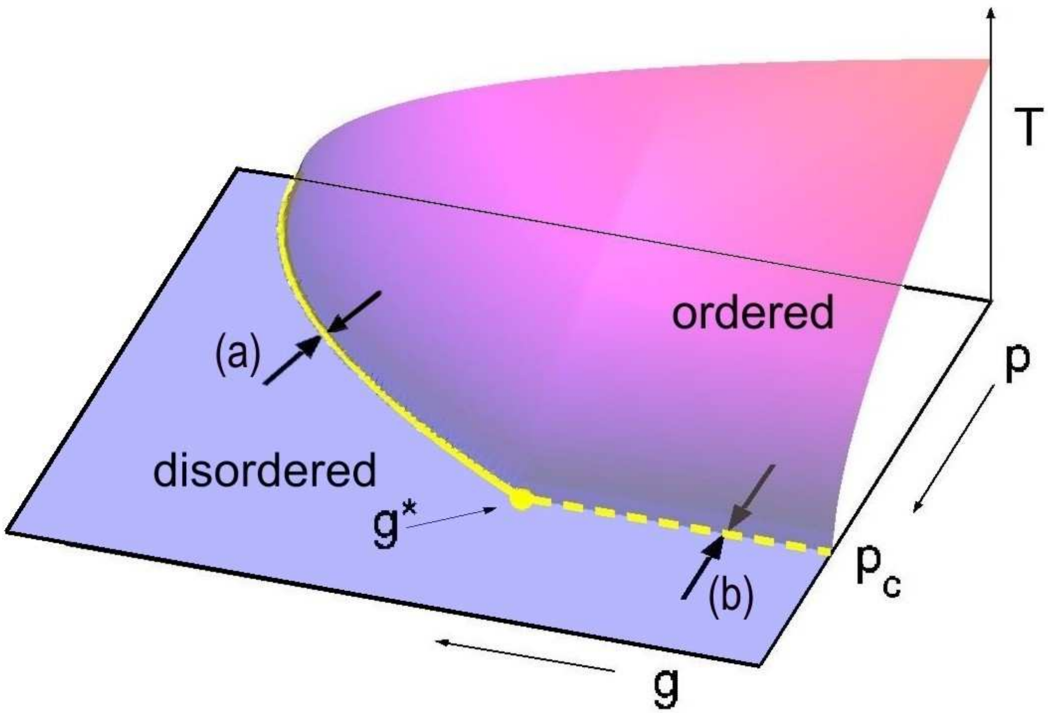
(if quantum fluctuations are not too strong)

⇒ phase diagram is of type (c)

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



Generic 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 $(g^*, p_c, T = 0)$

Critical behavior of percolation quantum phase transition

To determine the **critical behavior** of the percolation quantum phase transition:

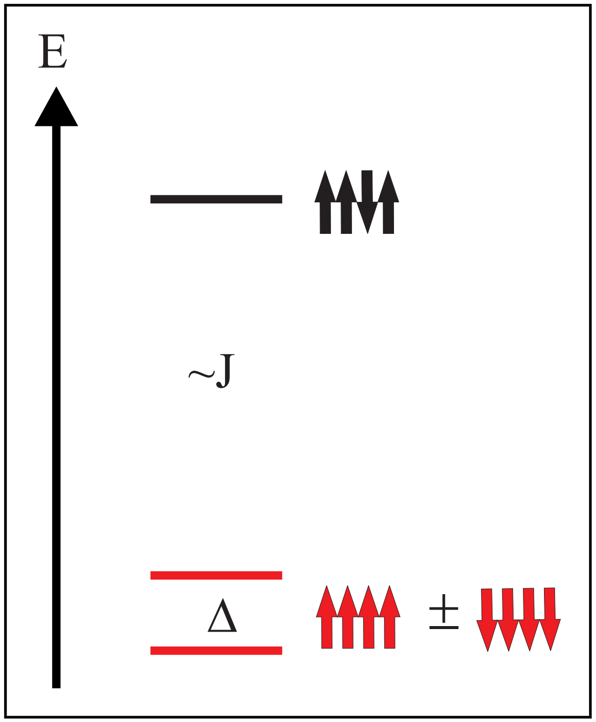
- first consider single percolation cluster,
- then combine **cluster size distribution** + **free energy of single cluster**

$$F_{\text{tot}} = \sum_s n_s(p - p_c)\, F_s$$

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 **two-level system** with moment s
- energy gap (inverse susceptibility) of cluster depends **exponentially** on size s

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



Critical behavior: Results

Static exponents are identical to classical lattice percolation exponents

- magnetization: long-range order on infinite cluster only $m \sim P_\infty \sim |p - p_c|^{\beta_c}$
- correlation length: correlations cannot extend beyond cluster size $\xi \sim \xi_c \sim |p - p_c|^{-\nu_c}$

Exponents involving dynamics are nonclassical

(but nonetheless determined by the lattice percolation exponents only)

- correlation time: $\ln \xi_\tau \sim \ln(1/\Delta) \sim s \sim \xi^{D_f} \Rightarrow$ activated scaling $\ln \xi_\tau \sim \xi^{D_f}$
- scaling form of the magnetization at the percolation transition (Senthil/Sachdev 96)

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

- 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 ζ

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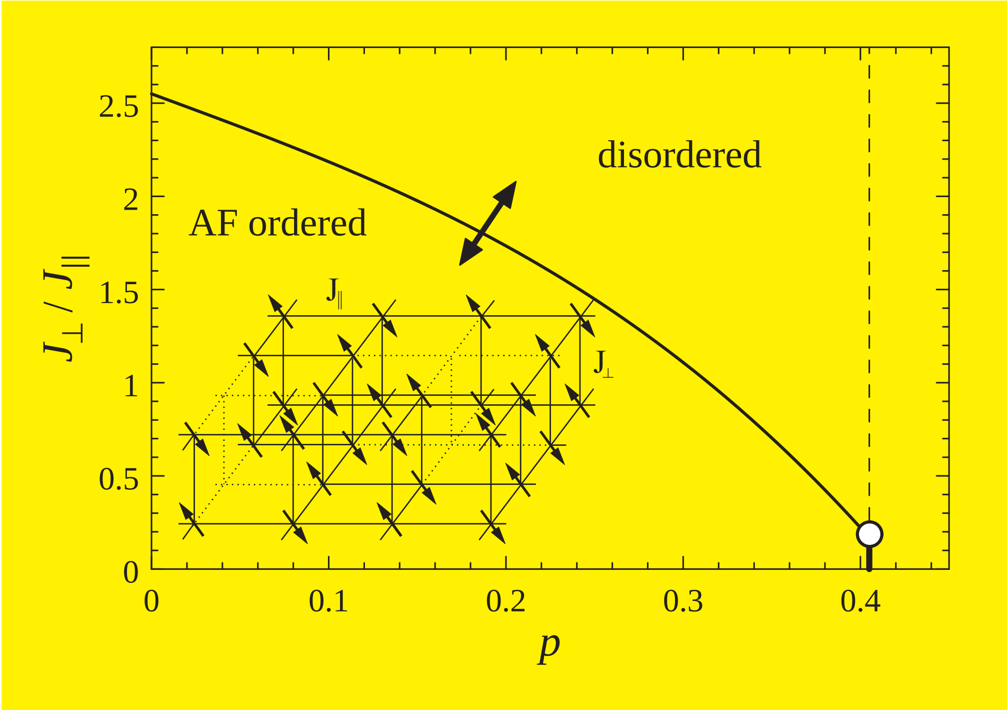
Diluted bilayer quantum Heisenberg antiferromagnet

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

- $\hat{\mathbf{S}}_{j,a}$: quantum spin operator ($S = 1/2$) at site j, layer a
- first term: in-plane interaction, second term: inter-layer coupling
- ratio $J_{\perp}/J_{\|}$ controls strength of **quantum** fluctuations



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

Nonlinear sigma model

bilayer antiferromagnet can be mapped to **quantum nonlinear sigma model** (NLSM)

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

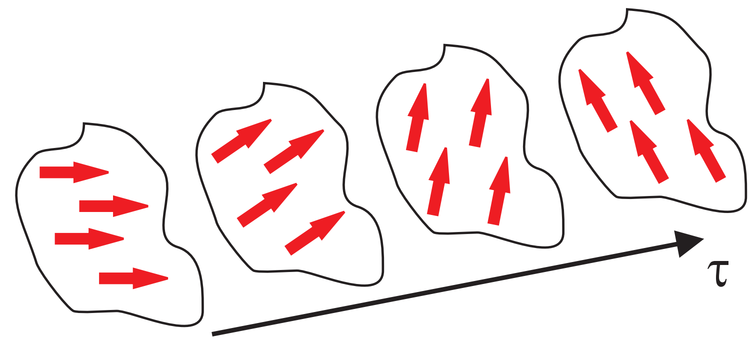
- $\mathbf{S}_i(\tau)$: N-component unit vector at site i and imaginary time τ
- $\epsilon_i = 0, 1$: random variable describing site dilution
- g strength of quantum fluctuations
- z_0: bare clean dynamic exponent, for bilayer antiferromagnet $z_0 = 1$

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

$\Rightarrow$ 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:

$$F_s\,(g,h,T) = (g^{\varphi}/s^{-\varphi})\Phi\left(hs^{1+\varphi}/g^{\varphi}, Ts^{\varphi}/g^{-\varphi}\right) \qquad \varphi = z_0/(2-z_0)$$

- free energy of quantum spin cluster more singular than that of classical spin cluster
- **susceptibility**: classically $\chi_s^c \sim s^2$, quantum (at $T=0$): $\chi_s \sim s^{2+\varphi}$
- **dynamical exponent** $z = \varphi D_f$ from $\chi_s \sim s^2/\Delta \Rightarrow \Delta \sim s^{-\varphi} \sim L^{-\varphi D_f}$

Critical behavior

Total free energy is sum over contributions of all percolation clusters

$$F_{\rm tot} = \sum_s n_s(p-p_c)\, F_s$$

General scaling scenario:

[T.V. + J. Schmalian, PRL **95**, 237206 (2005)]

$$\begin{aligned}
2-\alpha &= (d+z)\,\nu \\
\beta &= (d-D_f)\,\nu \\
\gamma &= (2D_f - d + z)\,\nu \\
\delta &= (D_f + z)/(d-D_f) \\
2-\eta &= 2D_f - d + z \; .
\end{aligned}$$

- exponents determined by lattice perc. exponents and **dynamical exponent** z
- **classical** exponents recovered for $z=0$:
- α, γ, δ, and η are **nonclassical** while β is **unchanged**

Exponents

Bilayer antiferromagnet:

$\varphi = 1 \quad \Rightarrow \quad z = D_f$

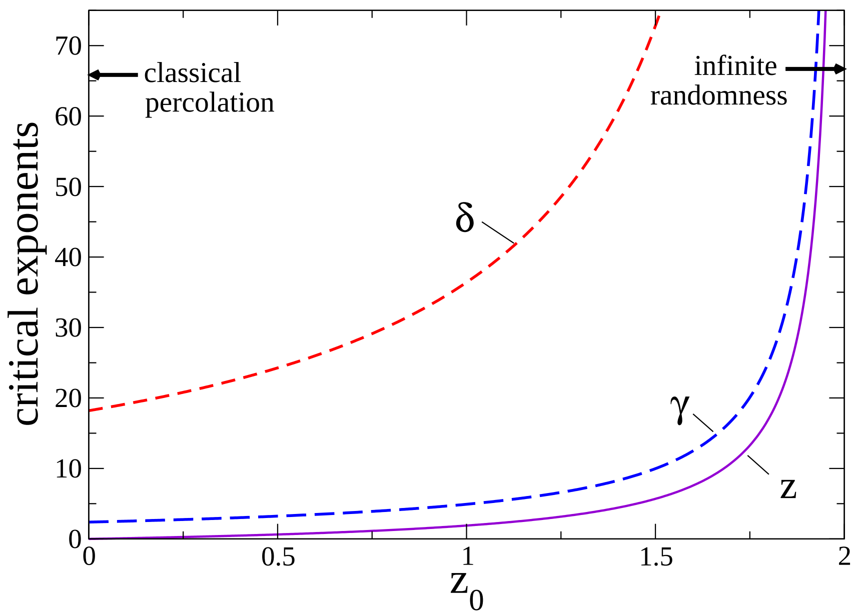
	2d		3d	
	classical	quantum	classical	quantum
α	$-2/3$	$-115/36$	-0.62	-2.83
β	$5/36$	$5/36$	0.417	0.417
γ	$43/18$	$59/12$	1.79	4.02
δ	$91/5$	$182/5$	5.38	10.76
ν	$4/3$	$4/3$	0.875	0.875
η	$5/24$	$-27/16$	-0.06	-2.59
z	-	$91/48$	-	2.53

Note: site diluted single layer:

- more complicated, Berry phases
- Sandvik + Wang: quantum MC
- value of z changes,

$z \approx (1.5 \ldots 2)\, D_f$

2D exponents as a function of z_0



- z diverges with $z_0 \to 2$
- $z_0 = 2$: activated scaling $\ln \Delta \sim L^{\psi}$
- $z_0 > 2$: clusters freeze, no quantum dynamics

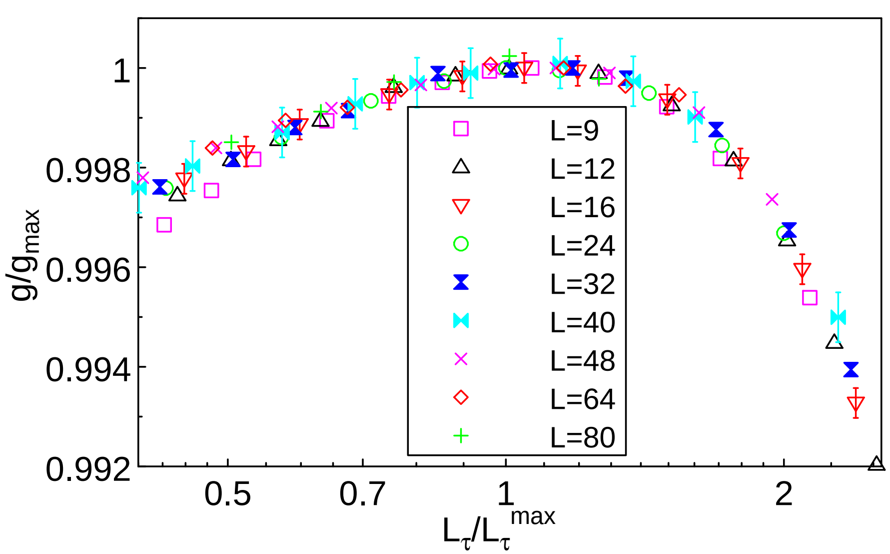
Monte-Carlo Simulation

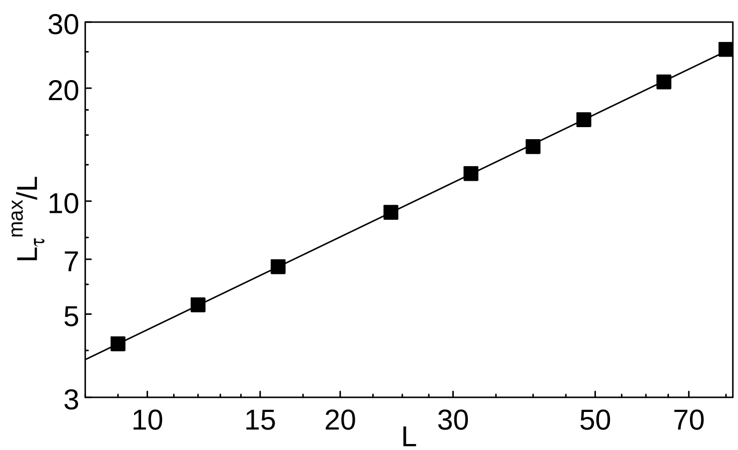
Quantum-to-classical mapping: 3D classical Heisenberg model with linear defects

$$H = K \sum_{\langle i,j \rangle,\tau} \epsilon_i \epsilon_j \mathbf{S}_{i,\tau} \cdot \mathbf{S}_{j,\tau} + K \sum_{i,\tau} \epsilon_i \mathbf{S}_{i,\tau} \cdot \mathbf{S}_{i,\tau+1},$$

- MC simulations of systems up to $120 \times 120 \times 2560$ sites
- several 10000 disorder realizations
- FSS of Binder cumulant at $p = p_c$ agrees well with theory

$\Rightarrow z \approx 1.83$



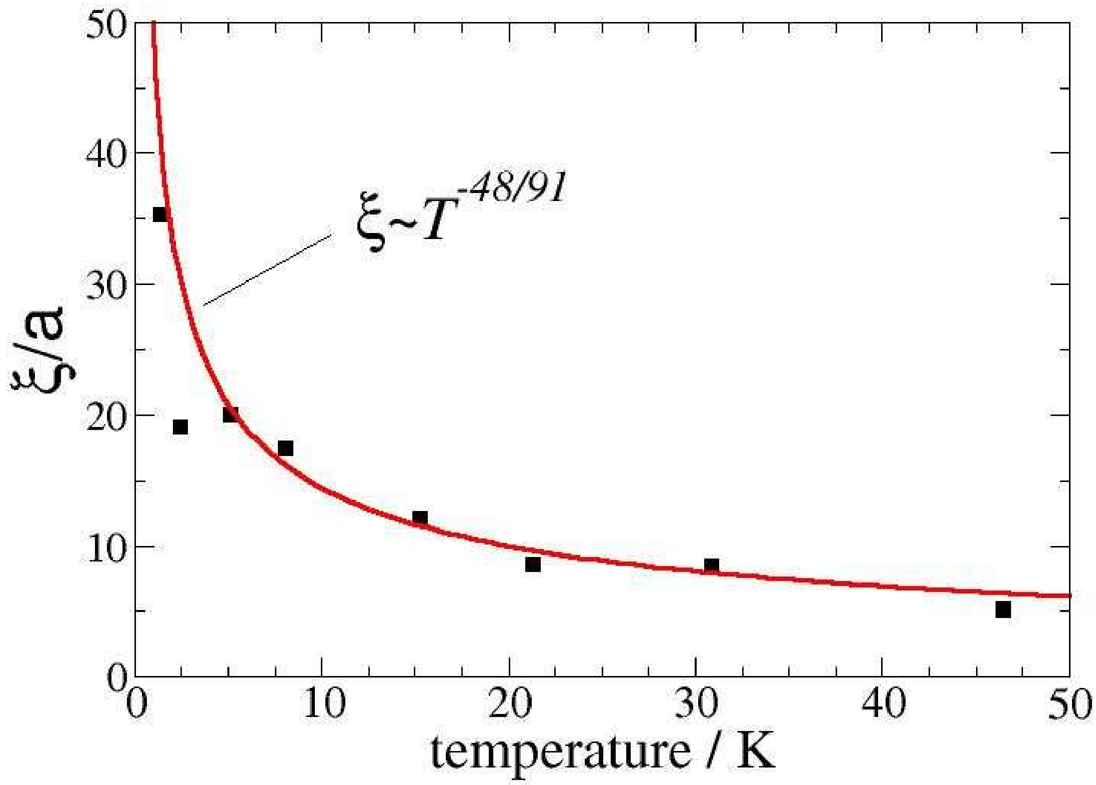


R. Sknepnek, M.V., T.V., PRL **93**, 097201 (2004), T.V., R. Sknepnek PRB **74**, 094415 (2006)

Experiment

Diluted Heisenberg antiferromagnet $La_2Cu_{1-x}(Zn,Mg)_xO_4$

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



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Dissipative transverse-field Ising model

- couple each spin to local bath of harmonic oscillators

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

- $a^\dagger_{i,n}, a_{i,n}$: 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

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

α dimensionless dissipation strength

ω_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**

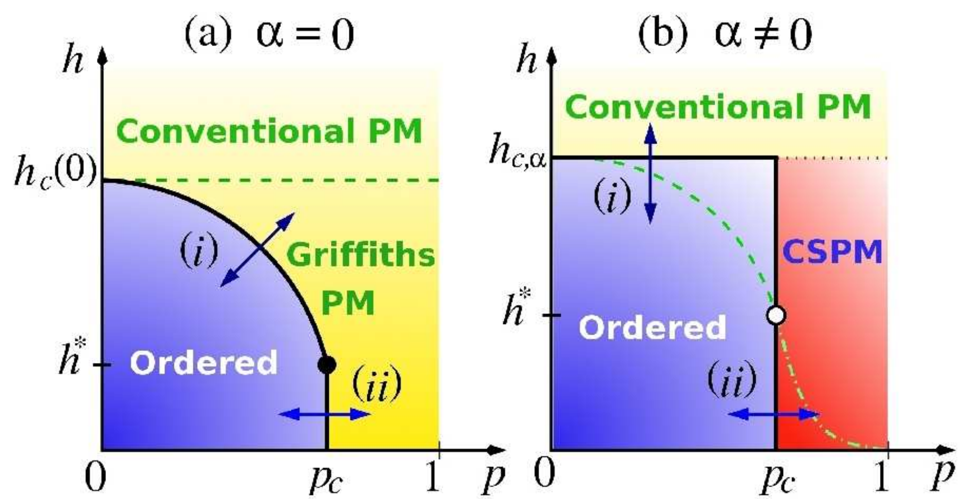
- frozen clusters act as classical superspins, dominate low-temperature susceptibility

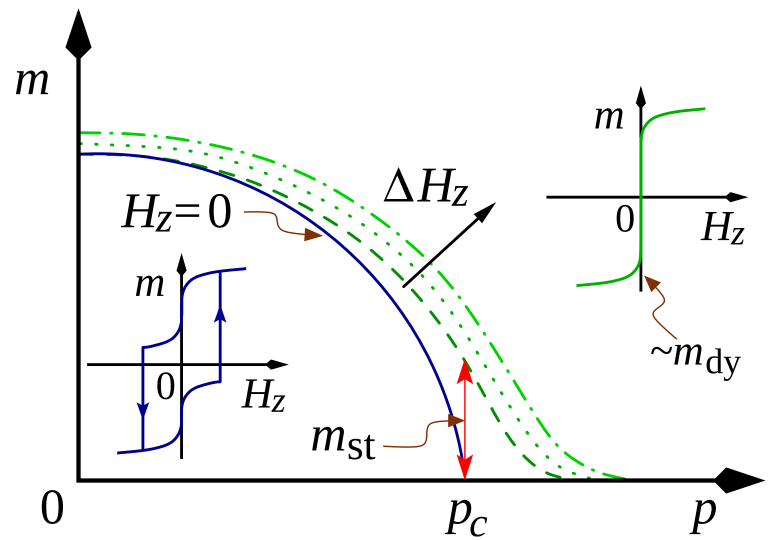
$$\chi \sim |p - p_c|^{-\gamma_c}/T$$

- 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**





J. Hoyos and T.V., PRB **74**, 140401(R) (2006)

Classification of dirty phase transitions according to importance of rare regions

Dimensionality of rare regions	Griffiths effects	Dirty critical point	Examples (classical PT, QPT, non-eq. PT)
$d_{RR} < d_c^-$	weak exponential	conv. finite disorder	class. magnet with point defects dilute bilayer Heisenberg model
$d_{RR} = d_c^-$	strong power-law	infinite randomness	Ising model with linear defects random quantum Ising model disordered directed percolation (DP)
$d_{RR} > d_c^-$	RR become static	smeared transition	Ising model with planar defects itinerant quantum Ising magnet DP with extended defects

Conclusions

- long-range order on critical percolation cluster is destroyed by thermal fluctuations
  long-range order survives a nonzero amount of quantum fluctuations
  $\Rightarrow$ 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 $\Rightarrow$ exotic transition, activated scaling

- Ohmic dissipation: large percolation clusters **freeze**, act as **superspins**
  $\Rightarrow$ **classical superparamagnetic cluster phase**

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