Quantum Magnetism and Quantum Criticality

- **• Classical and quantum phase transitions; RG and scaling**
- **• Finite-size scaling of simulation data**
- **• Example: dimerized Heisenberg models**
- **• J-Q models; valence-bond solids without QMC sign problem**
- **• Deconfined quantum criticality**

Finite-size scaling - "phenomenological RG"

Correlation length divergent for $T \to T_c$ $\xi \propto |\delta|^{-\nu}, \quad \delta = T - T_c$ Other singular quantity: $A(L \rightarrow \infty) \propto |\delta|^{\kappa} \propto \xi^{-\kappa/\nu}$ For **L-dependence** at T_c just let **ξ→L**: $A(T \approx T_c, L) \propto L^{-\kappa/\nu}$ Close to critical point: $A(L,T) = L^{-\kappa/\nu} g(\xi/L) = L^{-\kappa/\nu} f(\delta L^{1/\nu})$ Energy scale lowered with increasing system size; L is length scale at criticality

FIGURE 14. Monte Carlo results for the susceptibility (55) of the Ising model on several different *L*×*L*

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2D Ising universality class Critical T known \overline{a}

$$
T_c = 2/\text{ln}(1+\sqrt{2}) \approx 2.2692
$$

When these are not known, treat as fitting parameters - or extract in other way λ

Rough principles of renormalization

1) Kadanoff: Real-space blocking

Effective degrees of freedom of blocks reflect possible order parameters - interactions between blocks evolve to some fixed point

…) many other schemes, practical or mainly conceptual

Essence: an infinite number of effective couplings λ_i - flow as length scale is increased (energy scale is decreased): $\lambda_i(L) = \lambda_i^0 L_i^y$ Relevant ($y_i > 0$) or irrelevant ($y_i < 0$), λ_i^0 depends on model parameters - Very few relevant couplings ("fields")

Relevant and irrelevant perturbations of a critical point **influence Releva**

Critical correlation function of some operator Critical

M = *L^dm*. We ask whether this perturbation is relevant

$$
\langle O(\vec{r}_1)O(\vec{r}_2)\rangle = \sum_i a_i r^{-2\Delta_i}
$$

M = *L^dm*. We ask whether this perturbation is relevant

scaling dimension of *m*.

ordered state can also be stable or unstable under the

The scaling dimensions Δ_i correspond to the spectrum of 'orthogonal operators' (continuum fields) contained in the lattice operator O - Loosely speaking, we say that the smallest Δ_i is the scaling dimension of O Consider a critical Hamiltonian H₀ and add some pertu Consider a critical Hamiltonian H₀ and add some perturbation M \overline{h} corresponding to a phase of phase or phase the anti-- Loose for fixed values of *haired* in the lattice operator \overline{O} operators' (continuum fields) contained in the lattice of

stead vary the system size, which e↵ectively lowers the

$$
H = H_0 + h \sum_i m_i = hM \ (\equiv hNm = hL^dm)
$$

RG description of effects of hM at a critical point. Free energy density: **in RG** des

$$
f_s(t, h, L) = L^{-d} F_s(tL^{1/\nu}, hL^y)
$$

 $t-0$ at exitiaal point: e.g. $t-T$ Te (relevent fi - t=0 at critical point; e.g., t=1-1c (relevant field) $-t=0$ and $J_s(v, w, L) = L - I_s(vL, w, \theta)$
- t=0 at critical point; e.g., t=T-Tc (relevant field)

h $f_s^h \propto hL^{y-d}$ is $f_s^h \sim hL^{y-d}$ i Taylor

as *L* increases in the ordered phase. The cross-over length

than the conventional correlation length ⇠ / *|t|*

scale ⇠⁰ / *t*

From Hamiltonian: $f_s^h = h \langle m \rangle \propto h L^{-\Delta}$ y = s $From F$ p erturbation is $\begin{array}{ccc} \text{if } p & \text{if } p \neq 0 \\ \text{if } p & \text{if } p \neq 0 \end{array}$ we scaling dimension of h but, $s = h \sqrt{n} / \sqrt{n}$ if e the standard relationship $f h = h/m$ or $h I^{-\Delta}$ with From Hamiltonian: $J_s^v = n \langle m \rangle \propto nL$ \sim

- t=0 at critical point; e.g., t=T-Te (relevant field)
\nTavlor expand at t=0:
$$
f_s^h \propto hL^{y-d}
$$
 $\longrightarrow y = d - \Delta$

y = scaling dimension of h

⌫.

- The effect of the perturbation grows with the effect of the perturbation grows with \overline{I} (it is relevently \overline{I} perturbation if *y <* (a) with L (it is relevant and the critical point at the critical point is the critical point of α , the critical point at α , the critical point at α , the critical point at α , the critical - The effect of the perturbation grows with L (it is relevant) only if y>0
- *Irrelevant perturbation if y*<0 (the critical point stave the same) $-$ The - The effect of the perturbation grows with L (it is rel

than the conventional correlation length ⇠ / *|t|*

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- **perturbation if y <0 (the critical point if y <0 (the critical point if y <0 (the critical point is not if y <0 (the critical point is no in the state of the critical point is no in the state of the state of the state of** - Irrelevant perturbation if y<0 (the critical point stays the same) flow in a space of two or more of the space of the two or more of the
- A relevant perturbation changes the critic a but the case of the calculation in the case of a DIP, in the case of a DIP, it is equally because the critical point in so as *L* increases in the ordered phase. The cross-over length - inclusion perturbation in $y \sim ($ the onlineal point stays the same, $s = A$ rel

Symmetric and symmetry-breaking fields

Example: Ising model **Figure 2** and T critical point - classical model; energy and entropy At h=0, T tunes to the critical point - the 'thermal field' is $t=T-T_c$

Changing T changes the prefactor of E in

 $e^{-E(\sigma)/T}$

- E is the operators conjugate to T

$$
\langle E(r)E(0)\rangle \sim r^{-2\Delta_0}, \quad \Delta_0 = d - 1/\nu
$$

Set t=0, tune the magnetic field; $E \rightarrow E+hM$

-
$$
h \neq 0
$$
 breaks the Z_2 symmetry of the model; relevant but not symmetric

$$
\langle M(r)M(0)\rangle \sim r^{-2\Delta_M}, \ \ \Delta_M = d - 1/\nu_M
$$

The exponent Δ_M is related to the exponent we call η

$$
\langle M(r)M(0)\rangle \sim r^{-(d-2+\eta)} \qquad \Delta_M = (d-2+\eta)/2
$$

Normally systems have one relevant symmetric field

- multi-critical points have more than one

Gas-liquid transition

Maps to Ising model even though no apparent Ising (Z_2) symmetry Order parameter is density; scalar corresponds to <m> + constant

Tuning the relevant field corresponds to moving tangentially to the coexistence curve from the critical point (not so easy)

Tuning the symmetry-breaking field corresponds to moving perpendicularly to the coexistence curve

Moving along some generic path gives a mix of the two scaling dimensions in correlation functions; one eventually dominates

Example: O(3) transition in 2+1 dimensions (2D quantum) Examp sider the *S* = 1*/*2 bilayer Heisenberg Hamiltonian

Bilayer Bilayer Heisenberg model and the space (*the space of the space of the space of the space of the space* of the space o

the statistics.

croscopic interactions, until finally reaching a fixed point

$$
H=J_1\sum_{a=1,2}\sum_{\langle ij\rangle}S_{a,i}\cdot S_{a,j}+J_2\sum_{i=1}^NS_{1,i}\cdot S_{2,i} \qquad \qquad J_2\leftarrow I_3\leftarrow I_4\leftarrow I_5\leftarrow I_6\leftarrow I_7\leftarrow I_8\leftarrow I_9\leftarrow I_9\leftarrow I_9\leftarrow I_1\leftarrow I_2\leftarrow I_3\leftarrow I_1\leftarrow I_3\leftarrow I_4\leftarrow I_5\leftarrow I_6\leftarrow I_7\leftarrow I_7\leftarrow I_8\leftarrow I_9\leftarrow I_9\leftarrow I_9\leftarrow I_9\leftarrow I_1\leftarrow I_1\leftarrow I_1\leftarrow I_2\leftarrow I_3\leftarrow I_3\leftarrow I_1\leftarrow I_3\leftarrow I_1\leftarrow I_2\leftarrow I_3\leftarrow I_3\leftarrow I_1\leftarrow I_3\leftarrow I_4\leftarrow I_5\leftarrow I_1\leftarrow I_2\leftarrow I_3\leftarrow I_3\leftarrow I_4\leftarrow I_5\leftarrow I_5\leftarrow I_6\leftarrow I_7\leftarrow I_7\leftarrow I_7\leftarrow I_8\leftarrow I_7\leftarrow I_7\leftarrow I_8\leftarrow I_9\leftarrow I_9\leftarrow I_9\leftarrow I_9\leftarrow I_1\leftarrow I
$$

where *rij* denotes the separation of the sites *i* and *j*.

Critical at $J_2/J_1 \approx 2.5202$ C ritical of C $\frac{1}{4} \approx 2.5202$

The J_1 and J_2 terms are both relevant (no entropy at $T=0$)
- changing one of them takes us away from the critical point - changing one of them takes us away from the critical point $\overline{\text{The}} \cdot \text{Ina}$ - changi - changing one of them takes us away from the critical point are removed, not just the coupling between them). By tuning the coupling ratio *g* = *J*2*/J*¹ a coupling *J*2 (*I*² (*I*² (*I*² (*i*)² (*i* are removed, not just the coupling between them). By tuning the coupling ratio *g* = *J*2*/J*¹ a QPT can be reached for any dilution fraction *p<pc*, with *p^c* ⇡ 0*.*407 [8] being the classical Figure 1. The bilayer Heisenberg model with intraplane coupling *J*¹ (blue bonds) and interplane \overline{a} (*n*) \overline{a} (*red* vertical bonds). The open circles stand for removed dimers (i.e., the two spins). are removed, not just the coupling between them). By tuning the coupling ratio *g* = *J*2*/J*¹ a \Box point \Box $\mathfrak n$ point. \mathbf{F} is \mathbf{F} (blue bonds) and interpretation \mathbf{F} coupling *J*² (red vertical bonds). The open circles stand for removed dimers (i.e., the two spins are removed, not interesting the coupling ratio α QPT can be reached for any dilution fraction *p<pc*, with *p^c* ⇡ 0*.*407 [8] being the classical $\overline{1}$

trace out curves (MC RG flows) (*Q,*h*m*i)*^L* as *L* increases

 $\overline{J_1}$

*J*2

The Hamiltonian of the *S* = 1*/*2 spin model illustrated in Fig. 1 is give by

nearest-neighbor couplings [12] and the suscetibility was found to follow a stretched exponential to follow a
The suscetibility was found to follow a stretched exponential to form a stretched exponential to form a stretc

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h*ij*i

a=1*,*2

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i

a=1*,*2

h*ij*i

 J_2

).

Figure 1. The bilayer Heisenberg model with intraplane coupling *J*¹ (blue bonds) and interplane

*J*2

*J*1

*J*2

Binder ratios and cumulants

Consider the dimensionless ratio

 $R_2 =$ $\langle m^4 \rangle$ $\langle m^2 \rangle^2$

We know R₂ exactly for N→∞

• **for T<T_c:** $P(m) \rightarrow \delta(m-m^*) + \delta(m+m^*)$ m^* =|peak m-value|. $R_2 \rightarrow 1$ **• for T>T**_c: $P(m) \rightarrow exp[-m^2/a(N)]$

a(N)∼N-1 **R2→3** (Gaussian integrals)

The **Binder cumulant** is defined as (n-component order parameter; n=1 for Ising)

Systematic crossing-point analysis (2D Ising)

(b) The value of the cumulant at the crossing points, along with a fit to the form (11) for *L* 14.

Fit with L_{min} =12: T_c=2.2691855(5). Correct: T_c=2.2691853... to adapt the window size so that a relatively low order polynomial can be used. In the tests Figure 4: (a) Crossing temperature of the Binder cumulant for system-size pairs (*L,* 2*L*) versus the inverse of the smaller size, along with a fit to the form (10) to the data points with *L* 12.

reported here, cubic polynomials were used and all fits were statistically sound.

Correlation-length exponent

Consider some generic critical observable A

$$
A(L,t) = L^{-\kappa/\nu} f(\delta L^{1/\nu}) \rightarrow A(L,t)L^{\kappa/\nu} = f(\delta L^{1/\nu})
$$

Let us take the derivative wrt δ

$$
\frac{df(\delta L^{1/\nu})}{d\delta} = L^{1/\nu} f'(\delta L^{1/\nu}) \longrightarrow \frac{d(A L^{\kappa/\nu})}{d\delta} \propto L^{1/\nu} \quad (\delta = 0)
$$

The Binder cumulant is dimensionless

$$
U = U(\delta L^{1/\nu}, L^{-\omega_1}, L^{-\omega_2}, \ldots)
$$

$$
\frac{1}{\ln(2)} \ln \left(\frac{U'(2L)}{U'(L)} \right) \to \frac{1}{\nu}
$$

Test for 2D Ising $(\nu=1)$

Figure S3: Estimates of the inverse of the correlation-length exponent ⌫ of the 2D Ising model