Hysteresis and Dynamic Phase Transition in Kinetic Ising Models and Ultrathin Magnetic Films

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with many people over many years:

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Topic

Finite-size scaling study of dynamical phase transition in Ising ferromagnet below T_c, driven by oscillating field.

Differences from previous finite-size scaling studies of nonequilibrium phase transitions:

- Explicit time dependence in Hamiltonian.
- Both "ordered" and "disordered" states nonstationary in time and space.

Transition originally observed numerically.
(Lo, Pelcovits, Acharyya, Chakrabarti.)

Ingredients

- **Hysteresis.**
  Results from delayed response in systems subject to periodic applied force.
  - Example: Ferromagnet in oscillating field.
- **Finite-size scaling analysis of critical phenomena.**
  - Major method to analyze numerical data for systems undergoing phase transitions.
- **Decay of metastable phase.**
  Decay of a metastable phase in a spatially extended physical system, driven by thermal nucleation and subsequent growth of droplets.
  - For large systems well described by the Kolmogorov-Johnson-Mehl-Avrami (KJMA) theory.

Model

2D Ising Hamiltonian on $L \times L$ square lattice:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - H(t) \sum_{i}^{L^2} s_i$$

Dimensionless magnetization:

$$m = L^{-2} \sum_i s_i$$

Temperature $T < T_c \Rightarrow m$ for $H{=}0$ takes one of two degenerate equilibrium values:

$$m(T < T_c,\ H{=}0) \ = \ \pm m_{\mathrm{eq}}(T)$$

Stochastic dynamic

Glauber (nonconserved) dynamic with transition probability

$$W(s_i \to -s_i) = \frac{\exp(-\beta \Delta E_i)}{1 + \exp(-\beta \Delta E_i)}$$

where ΔE_i is the proposed energy change.

KJMA (Avrami) theory of metastable decay

Following sudden field reversal, critical droplets nucleate at constant rate per unit volume

$$I(T,H) \propto \exp\left[-\frac{\Xi(T)}{k_{\mathrm{B}} T H^{d-1}}\right]$$

Large supercritical droplets grow

at constant velocity

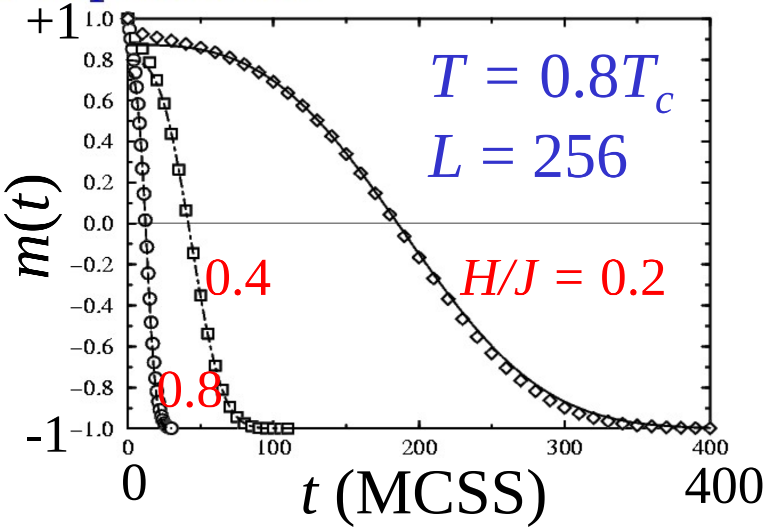
$$v \propto |H|$$

Time evolution of magnetization in KJMA theory

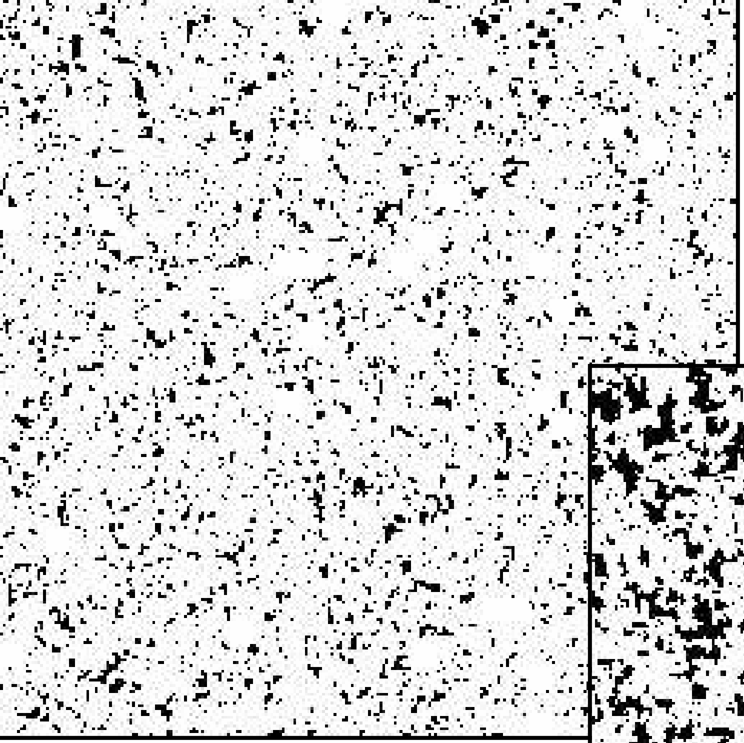
(randomly placed, freely overlapping droplets):

$$m(t) \approx m_{\rm eq}(T)\left\{2\exp\left[-I\int_0^t \Omega_d (vs)^d {\rm d}s\right]-1\right\}$$
$$= m_{\rm eq}(T)\left\{2\exp\left[-\frac{\Omega_d}{d+1}\left(\frac{t}{\tau}\right)^{d+1}\right]-1\right\}$$

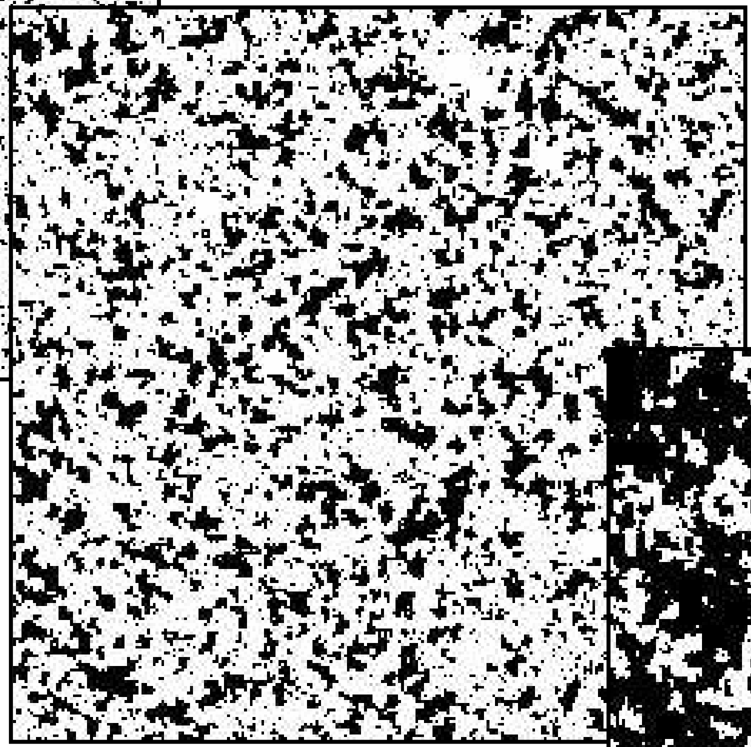
$\langle\tau\rangle = (v^d I)^{-\frac{1}{d+1}}$ is average metastable lifetime. $R_0 \approx v\langle\tau\rangle$ is average droplet separation.



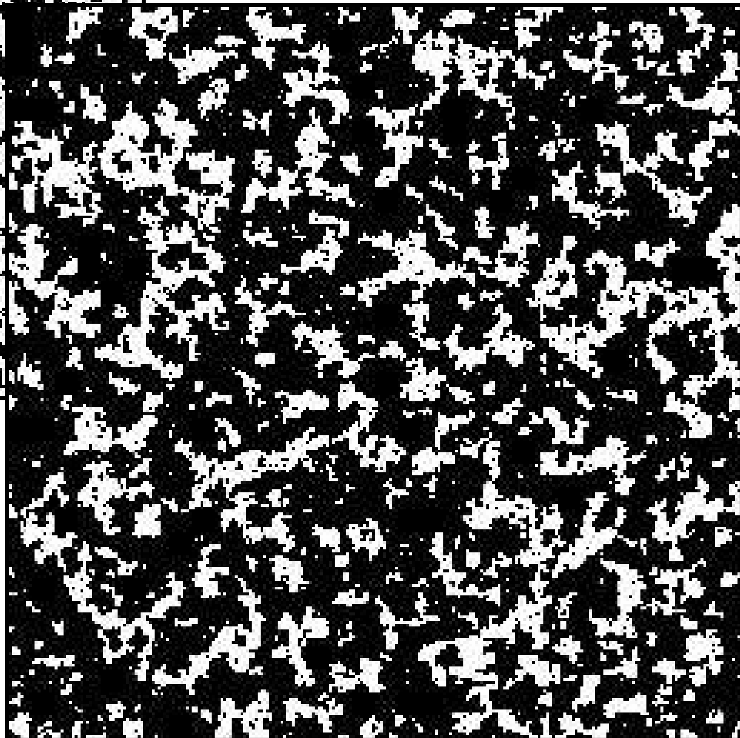
Snapshots



$\Theta = 0.1$



$\Theta = 0.3$



$\Theta = 0.7$

Hysteresis

Apply oscillating field,

$$\text{Commonly:} \quad H(t) = H_0 \sin(\pi t / t_{1/2})$$

$$\text{Or square wave:} \quad H(t) = H_0 (-1)^{\text{int}(t/t_{1/2})}$$

Time-dependent nucleation rate in adiabatic limit:

$$I\left(T, H(t)\right) \propto \exp\left[-\frac{\Xi(T)}{k_{\text{B}} T H(t)^{d-1}}\right]$$

and interface velocity

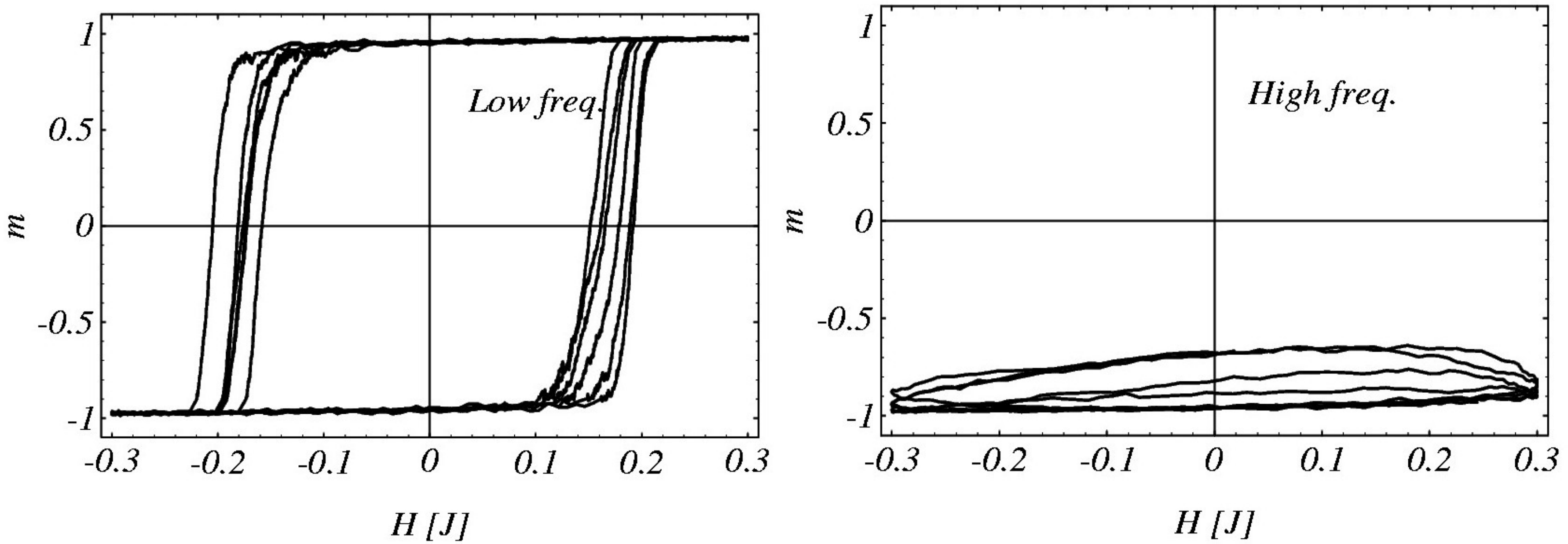
$$v\left(H(t)\right) \propto |H(t)|$$

Scaled field period:

$$\Theta = \frac{\text{field half} - \text{period}}{\text{metastable lifetime}} = \frac{t_{1/2}}{\langle \tau(H_0, T) \rangle}$$

Symmetry breaking in oscillating field

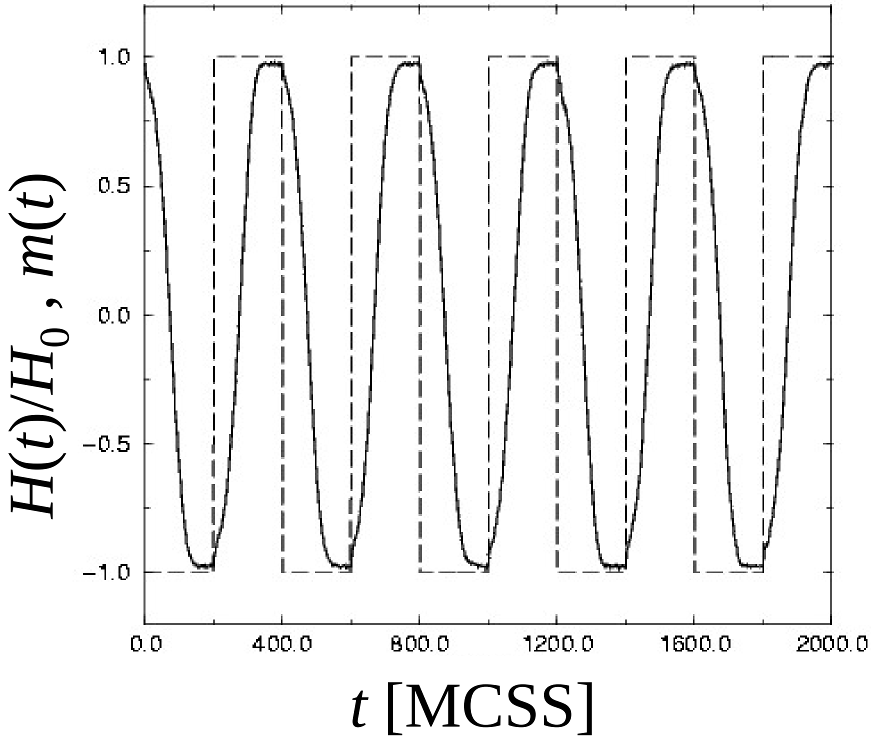
Ising model in sinusoidal field at $0.8T_c$

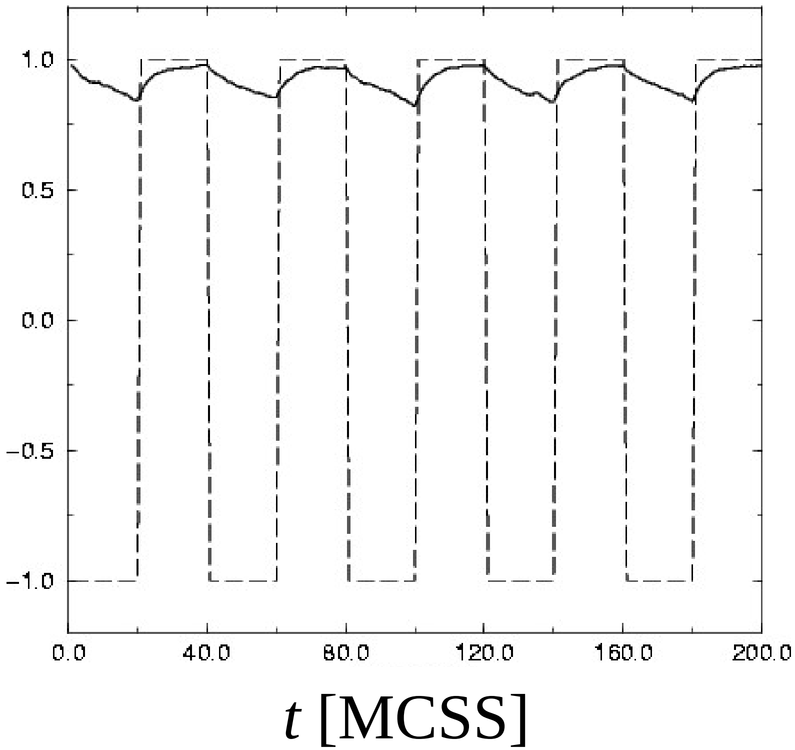


Dynamic phase transition
(Square-wave field)

$T = 0.8T_c$, $H_0 = 0.3J$

Low frequency High frequency





Symmetry breaking!

Square-wave Field: Simulation Details

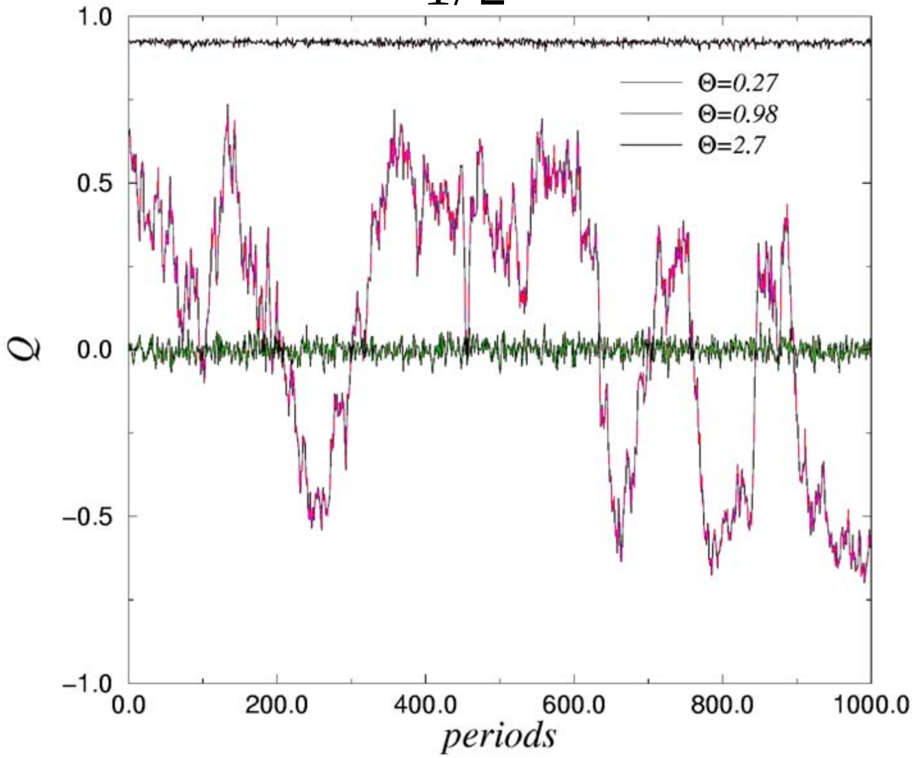
1. **Parameters**
   - Temperature: $T{=}0.8T_c$
   - Square lattice, $L{=}64$, 90, 128, 256, 512
   - Applied square-wave field:
     $H(t) = H_0(-1)^{\mathrm{int}(t/t_{1/2})}$, $H_0 = 0.3J$.
   - Lifetime: $\langle\tau(H = H_0, T)\rangle = 75$
   - Droplet separation: $R_0 \approx 10$
   - Dimensionless field period: $\Theta{=}\ \frac{t_{1/2}}{\langle\tau(H_0,T)\rangle}$
   - Run lengths: $0.3 - 1.5 \times 10^7$ MCSS

2. **Analysis**
   - Period-averaged magnetization: $Q = \frac{1}{2t_{1/2}} \oint m(t)\mathrm{d}t$

     is the dynamic order parameter

Analyze the period-averaged order parameter

$$Q = \frac{1}{2t_{1/2}} \oint m(t)\mathrm{d}t$$

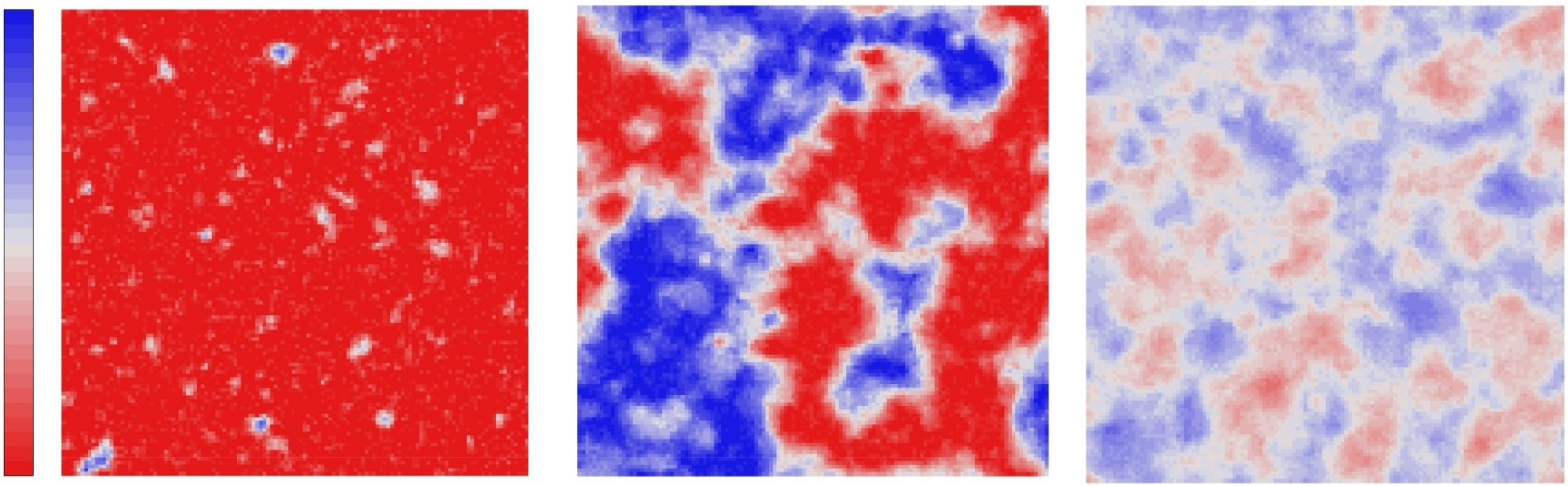


Dimensionless period: *Θ = Half-period/Lifetime*

$T = 0.8T_c$, $H_0 = 0.3J$

Configurations of local Q_i

$$T = 0.8T_c\ ,\ H_0 = 0.3J\ ,\ L\ =\ 128$$



$\Theta = 0.27 < \Theta_c$ — Ordered

$\Theta = 0.98 \sim \Theta_c$ — Critical

$\Theta = 2.7 > \Theta_c$ — Disordered

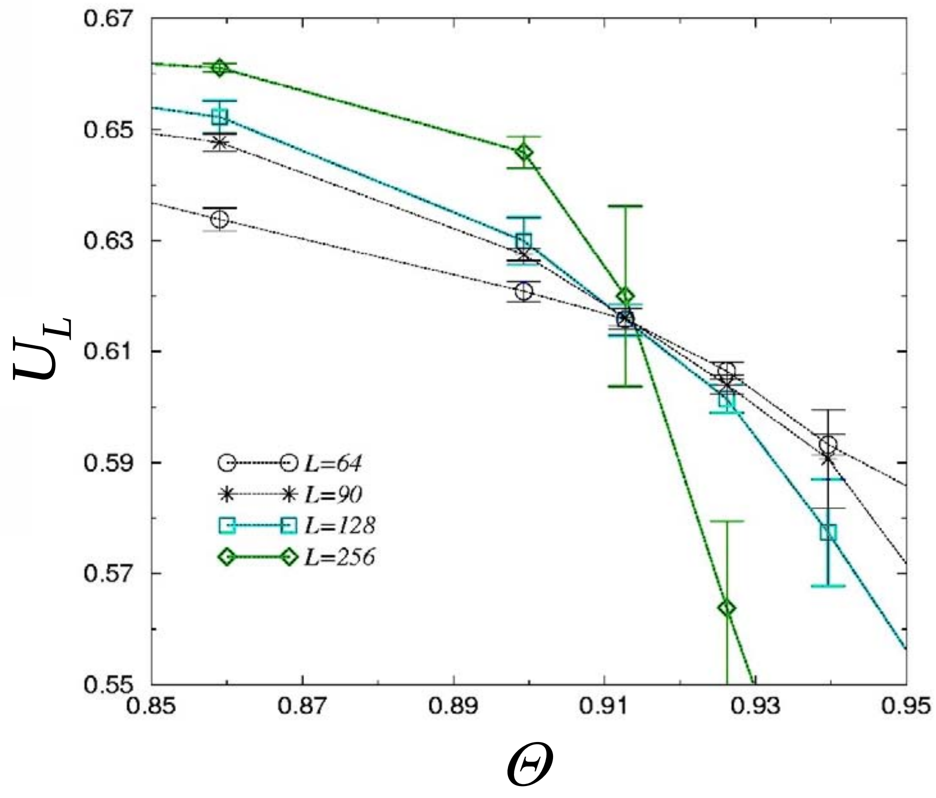
Finite-size scaling

Fourth-order cumulant ratio

$$U_L = 1 - \frac{\langle |Q|^4 \rangle_L}{3\langle |Q|^2 \rangle_L^2}$$

Describes shape of order-parameter distribution. Fixed point

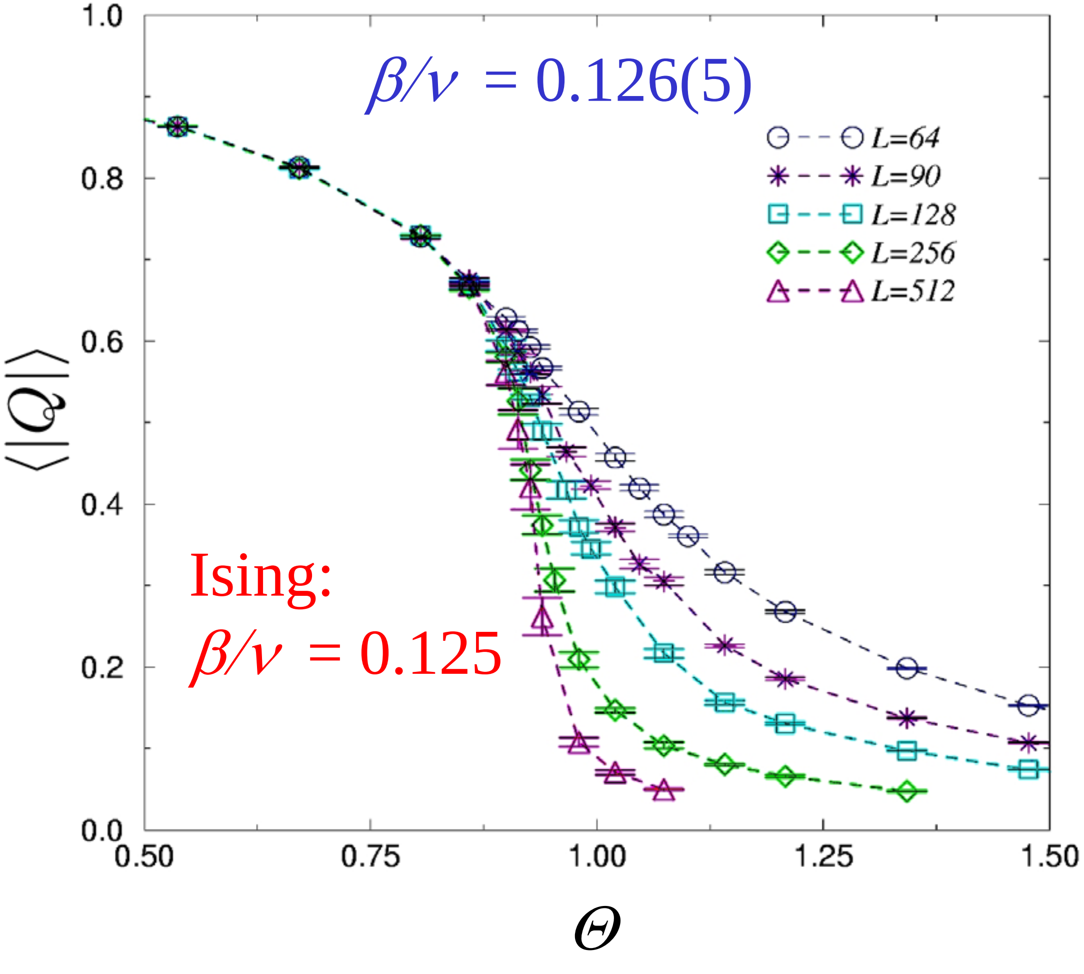
$U^* = 0.611(3)$, $\Theta_c = 0.918(5)$



Order parameter vs Θ

$T = 0.8T_c$, $H_0 = 0.3J$

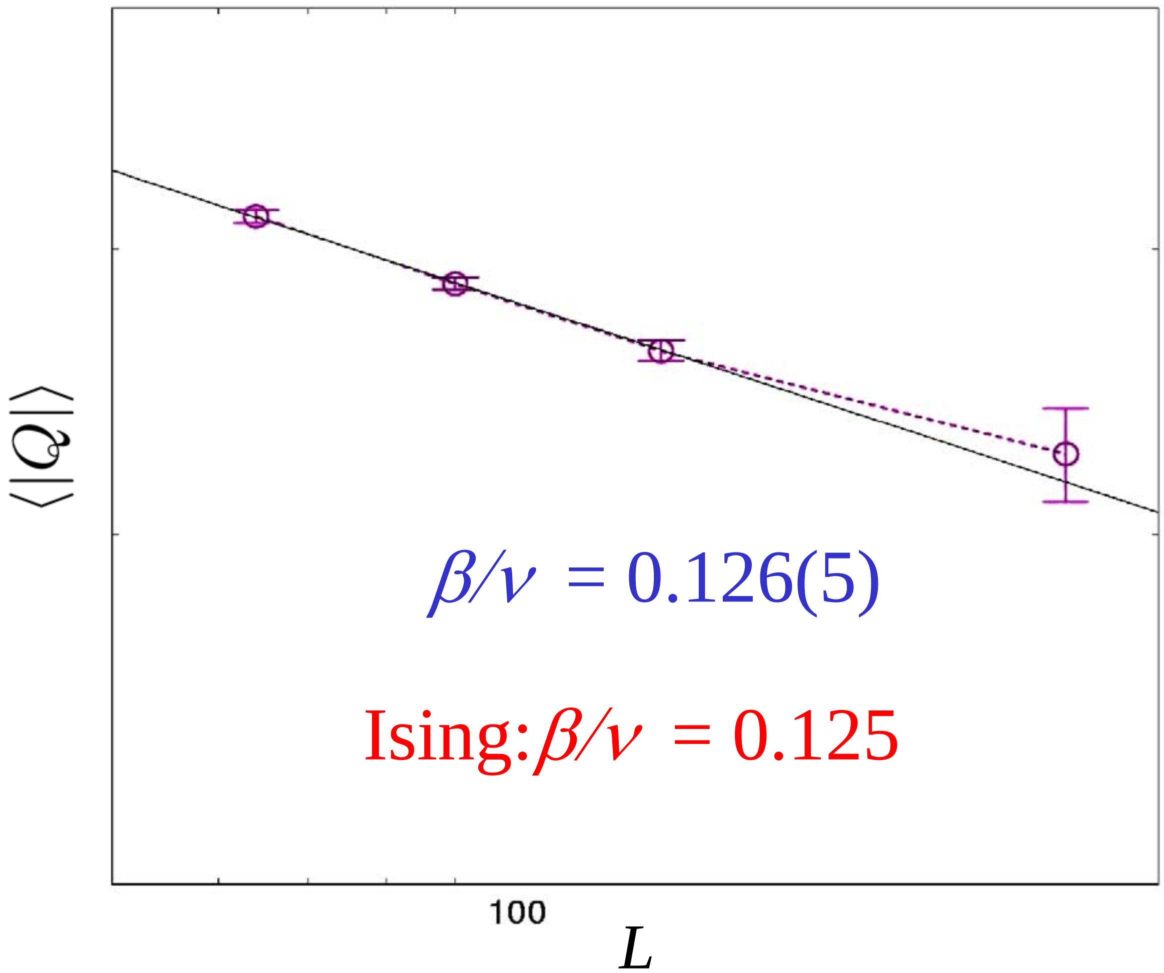
Scaling relation: $|Q(\Theta_c)| \sim L^{-\beta/\nu}$



Scaling plot for β/ν

Scaling relation

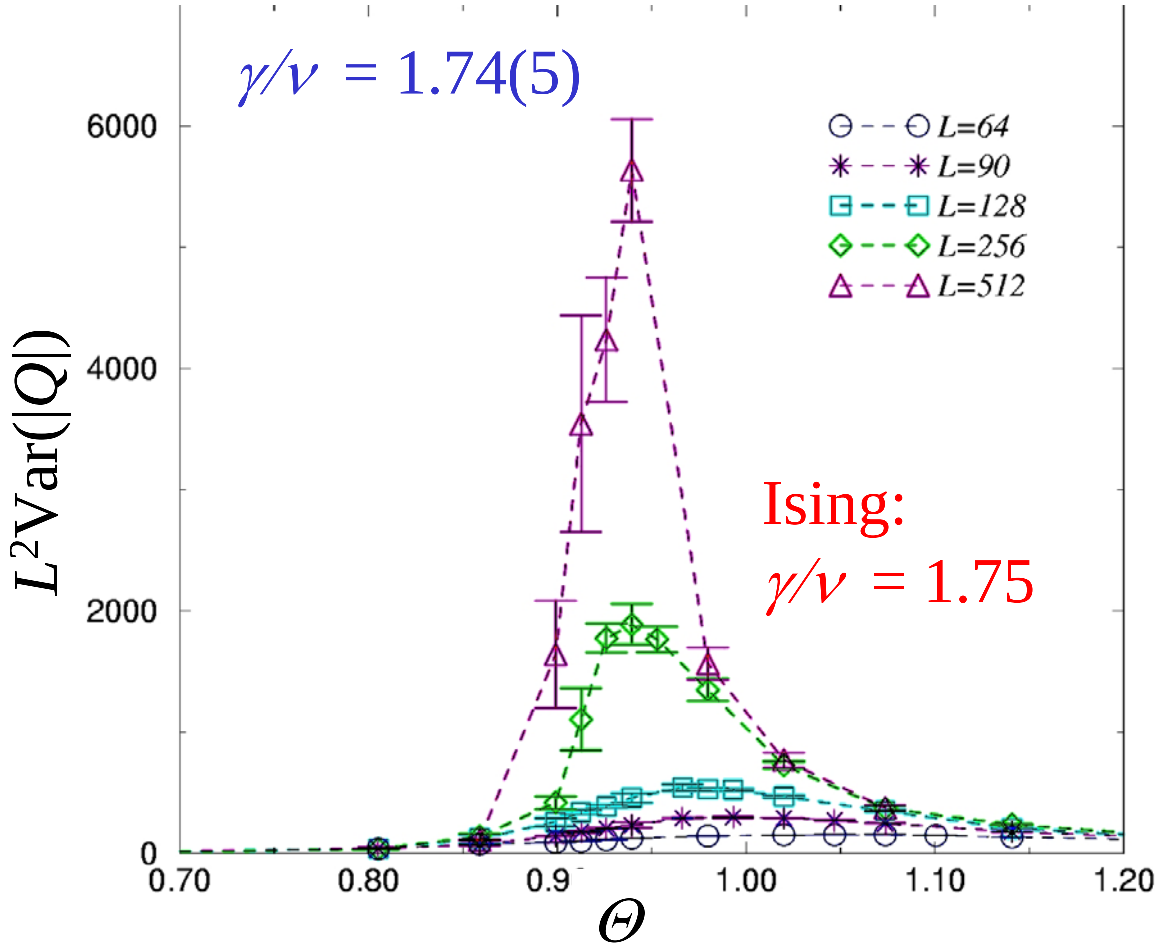
$$\langle |Q(\Theta_c)| \rangle \propto L^{-\beta/\nu}$$



Order-parameter fluctuations vs Θ

$$T = 0.8T_c\ ,\ H_0 = 0.3J$$

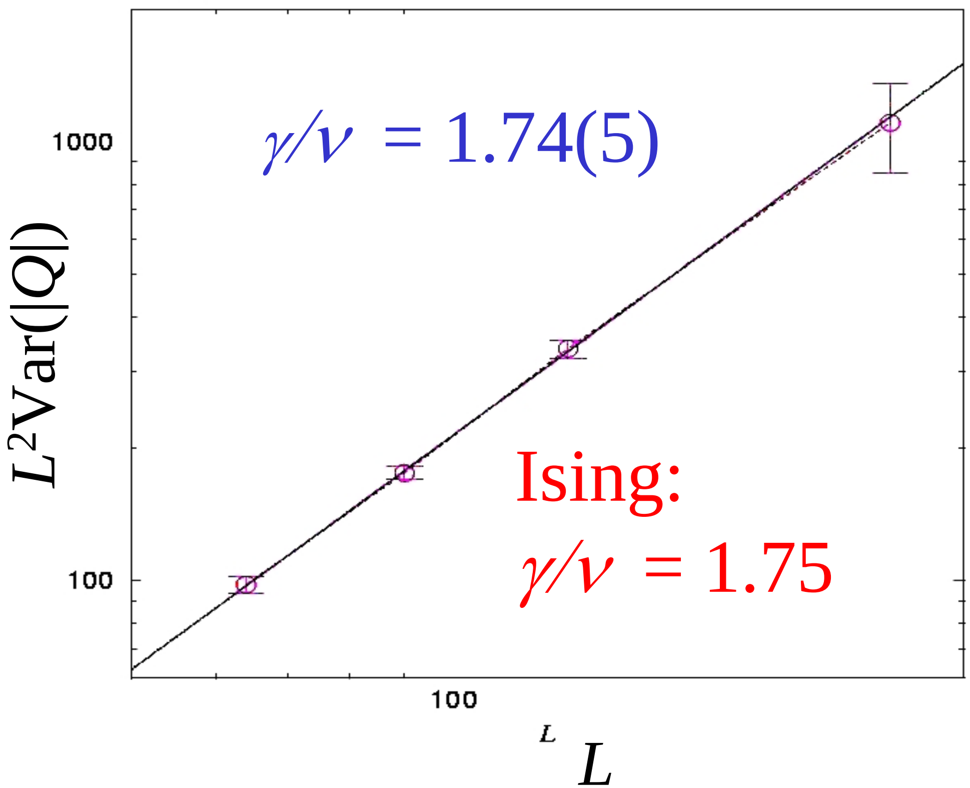
Scaling relation at Θ_c: $X = L^2\mathrm{Var}(|Q|) \sim L^{\gamma/\nu}$

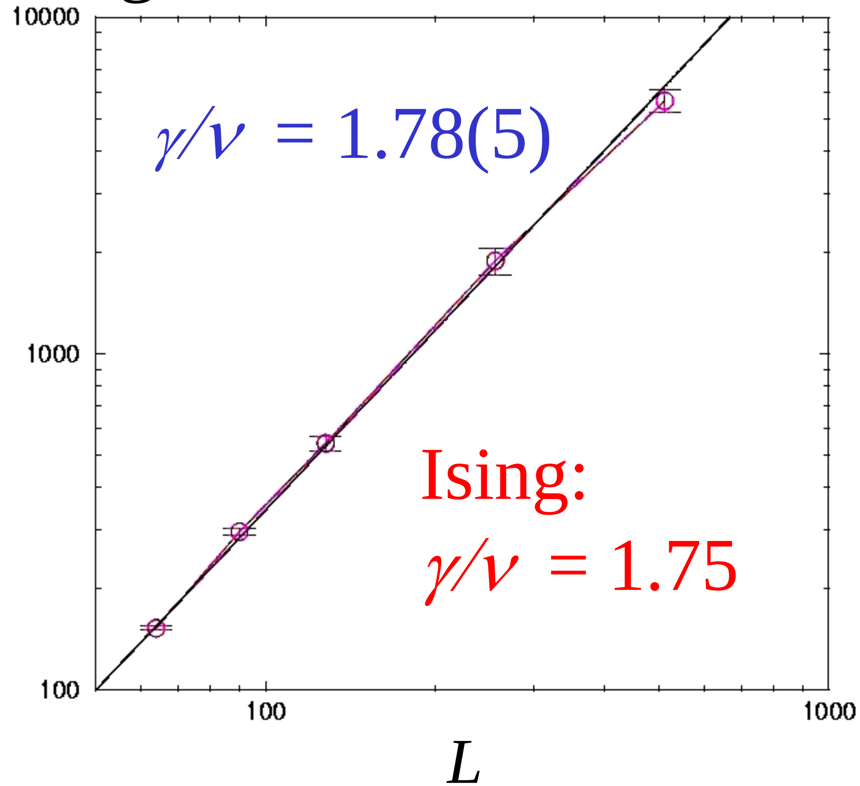


Scaling plot for γ/ν

$$X = L^2 \mathrm{Var}(|Q|) = L^2 \left[\langle |Q|^2 \rangle - \langle |Q| \rangle^2 \right] \propto L^{\gamma/\nu}$$

Using fluctuations at Θ_c : Using fluctuations at maximum

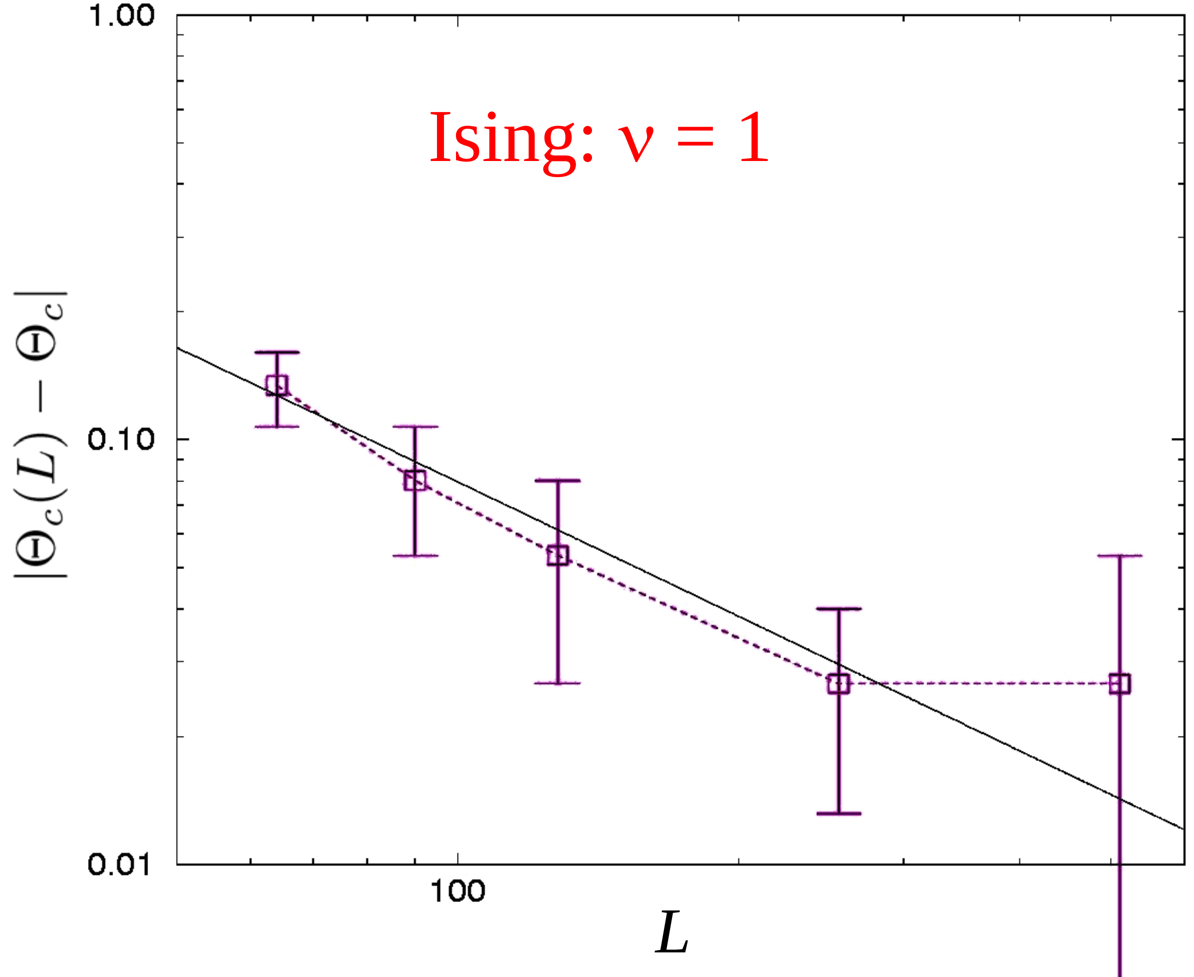




Scaling plot for $1/\nu$

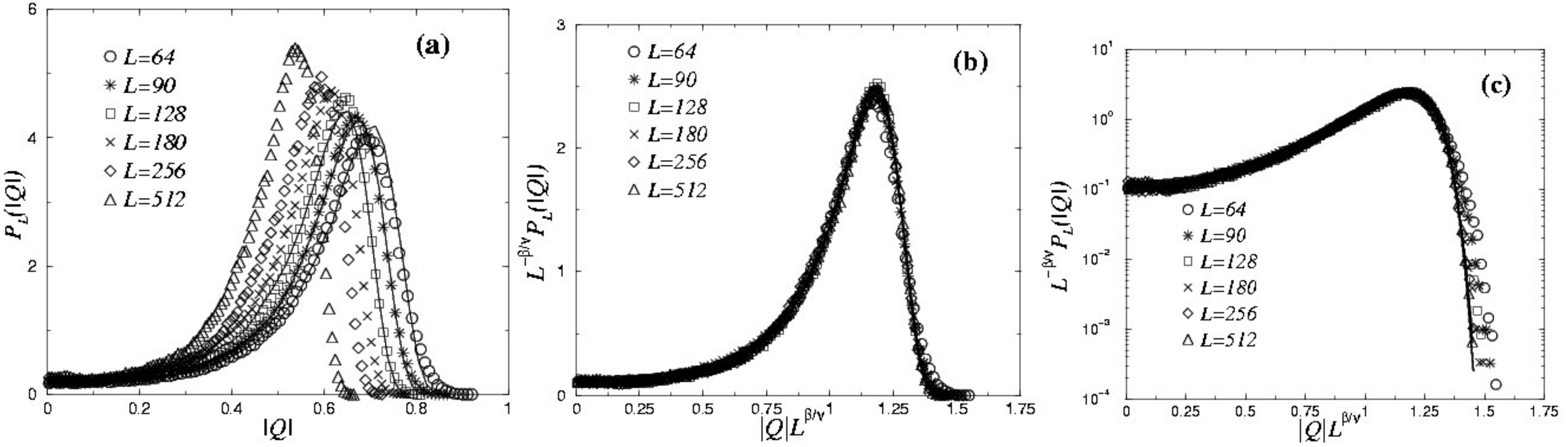
$$|\Theta_{\rm max} - \Theta_{\rm c}| \propto L^{-1/\nu}$$

yields $\nu = \mathbf{0.95} \pm \mathbf{0.15}$



Scaling of order-parameter distribution, $P_L(|Q|)$

Scaling with Ising exponents, $\beta/\nu = 1/8$



Unscaled Scaled Lin/Log

Conclusion: This nonequilibrium phase transition is in the equilibrium Ising universality class!!

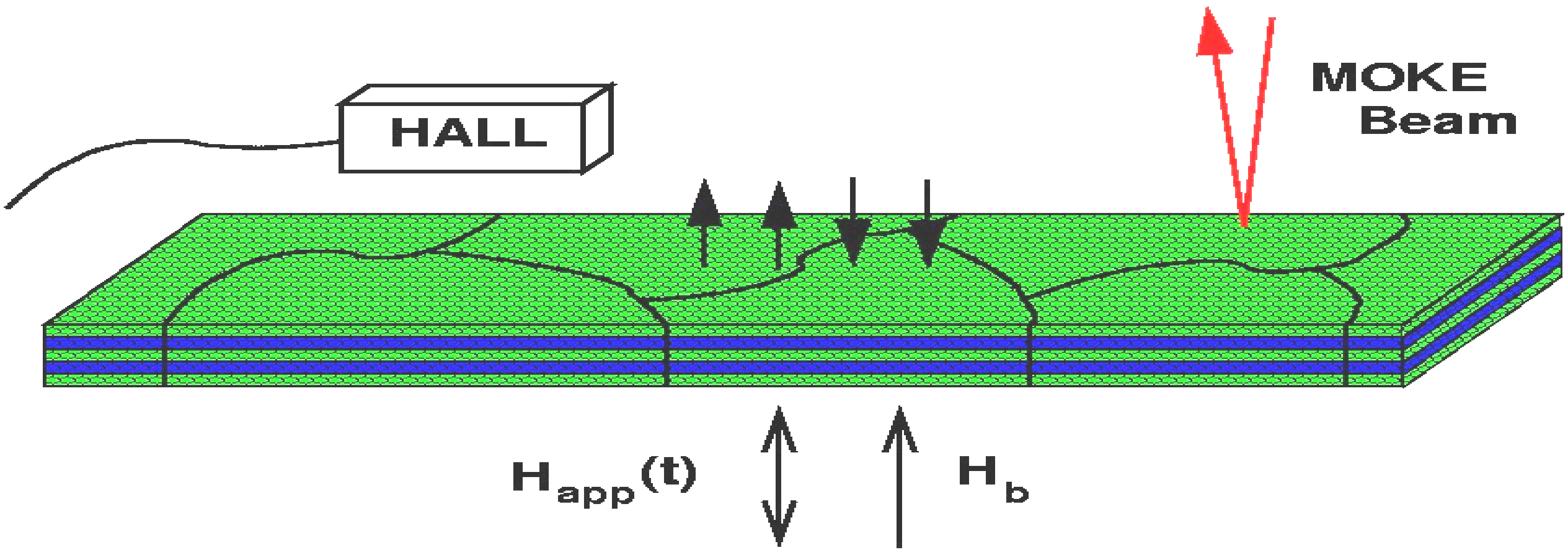
(Confirmed analytically, Fujisaka, Tutu, Rikvold PRE **63**, 036109 (2001))

Experimental observation

$[Co/Pt]_3$ multilayer under oscillating field with nonzero *bias*

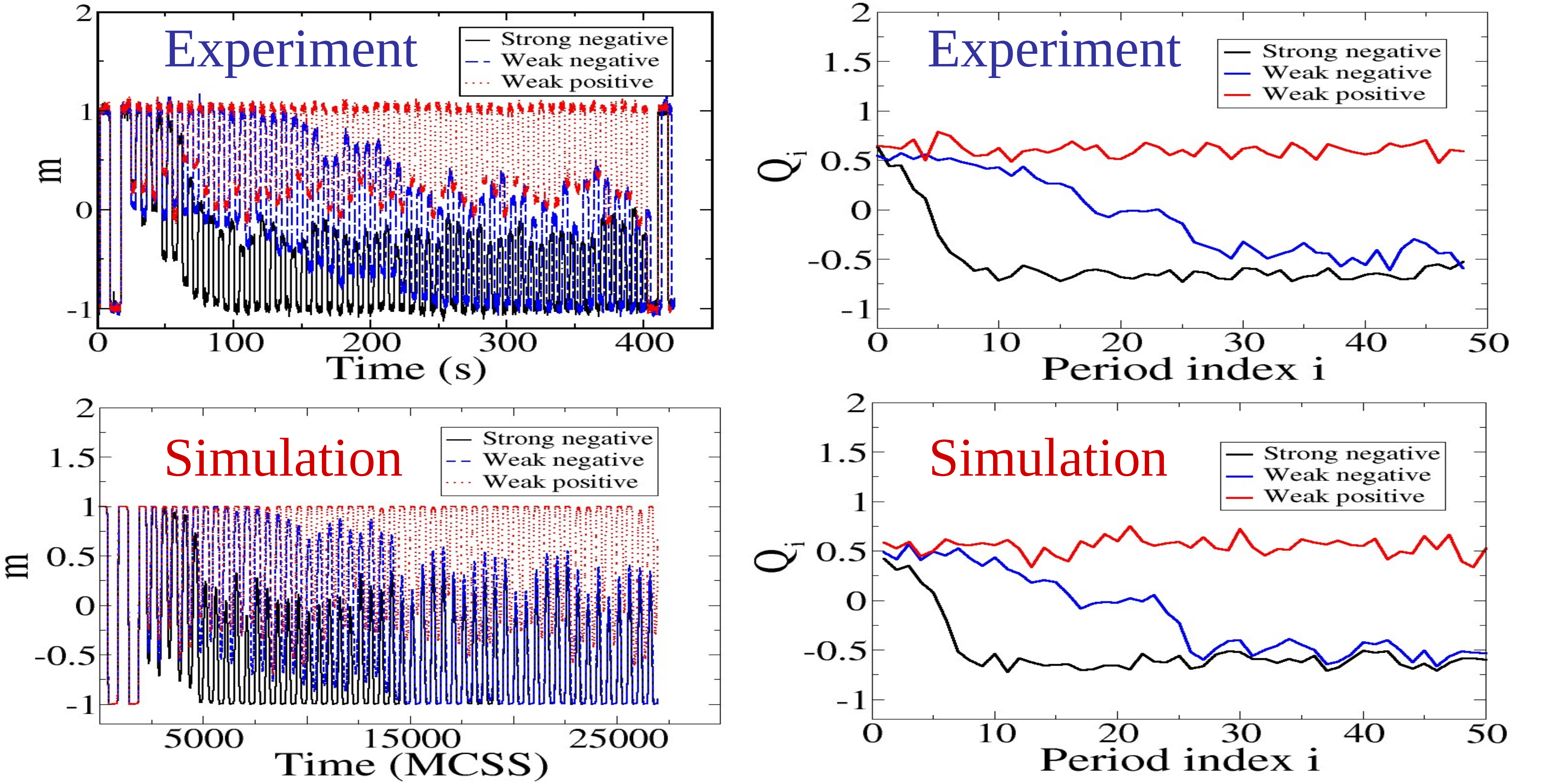
D. T. Robb et al., Phys. Rev. B **78**, 134422 (2008)

Experimental multilayer system (A. Berger, D. T. Robb, et al.)



- [Co(0.4nm) / Pt(0.7 nm)]$_3$ multilayer. Lateral grain size: 30-300 nm
- Strong perpendicular anisotropy
  → Little effect from demagnetizing field
- Apply out-of-plane periodic magnetic field with electromagnet, as well as small constant "bias field" of varying strength
- Measure magnetic field with Hall probe, and magnetization response with MOKE (Magneto-Optic Kerr Effect) beam (spot size ≈ 1 mm^2)

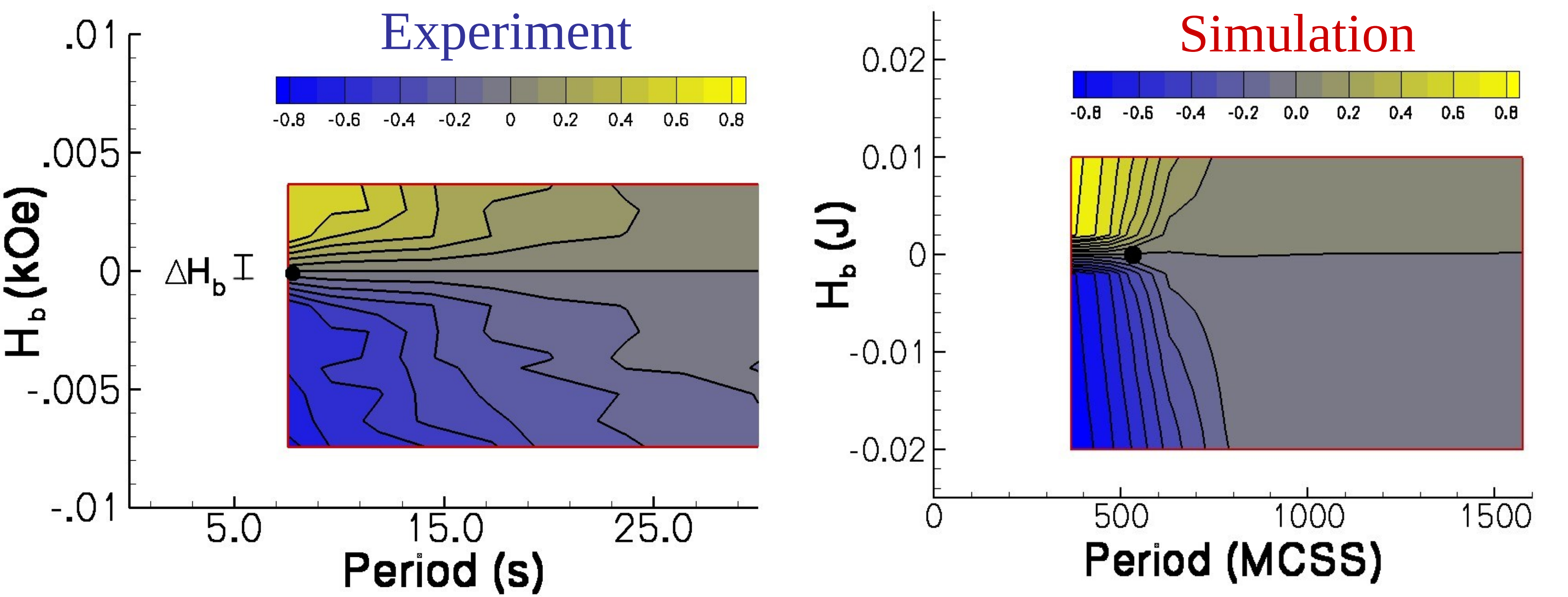
Experimental evidence for DPT : metastable state



- **Q_i vs i in experiment at $P = 7.6\ s$, in varying bias fields. Similar to Q_i *vs* i in simulation at $P = 500\ MCSS = 0.95P_c$ (with comparable bias)**

- **Metastable dynamically ordered state in weak *negative* bias field**

Evidence for DPT: non-equilibrium phase diagram



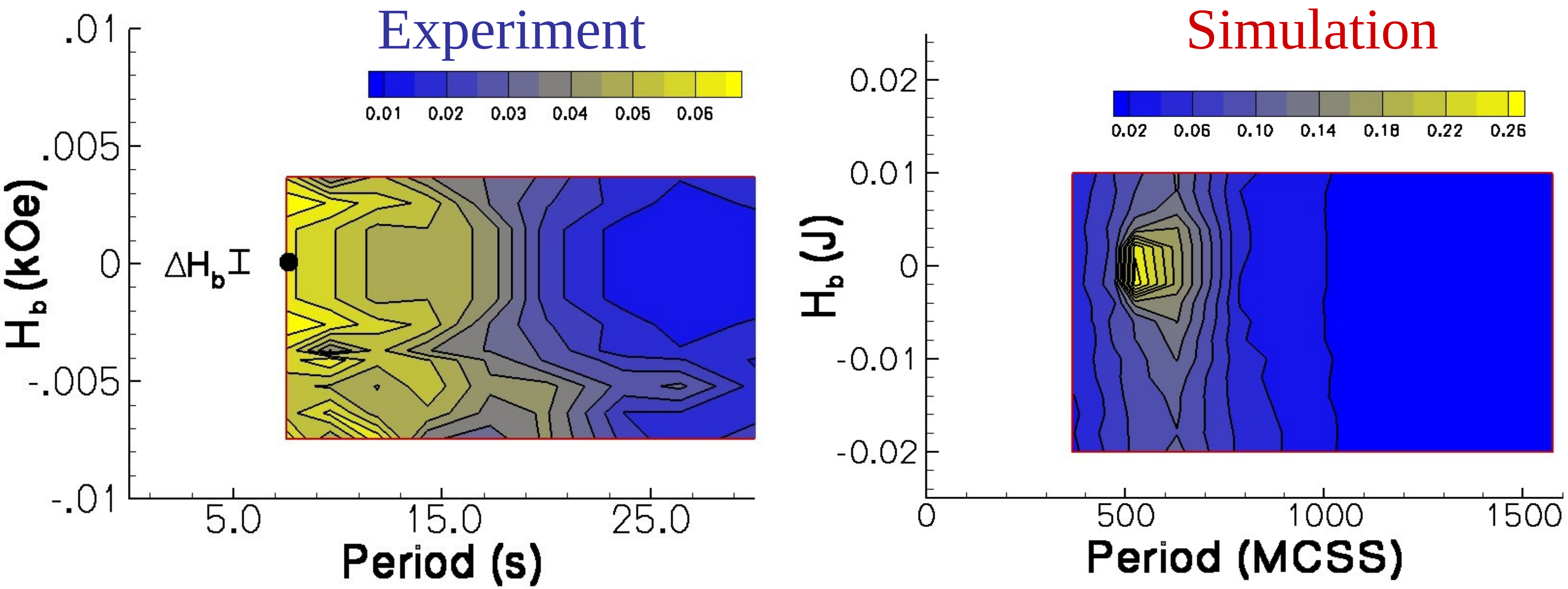
- **Characterize response by non-equilibrium phase diagram (NEPD)**

  $\langle Q_i \rangle (P, H_b)$**, in analogy with equilibrium phase diagram** $\langle m \rangle (T, H)$

- **Similarity: large change in** $\langle Q_i \rangle$ **over small range of** H_b **as** $P \rightarrow P_{c+}$

- **Difference: greater impact of a given bias field for** $P > P_c$ **in experiment (believed to be caused by pinning in reversal process)**

Fluctuations in non-equilibrium steady state



- **In equilibrium Ising system, fluctuations $\sigma_m(T, H)$ increase as $T \to T_c$ and $H \to 0$**
- **By analogy, near DPT in kinetic Ising simulation, $\sigma_Q(T, H)$ increases as $P \to P_c$ and $H_b \to 0$: similar trend in experiment**

Natural questions about the DPT

1. Given the experimental results, is there a field H_c conjugate to Q, analogous to the magnetic field H in the equilibrium Ising model?

A: Yes, the period-averaged magnetic field ('bias field') H_b, as suggested by the recent experiments on [Co/Pt]-multilayers, is the conjugate field H_c.

2. In the equilibrium Ising system, a fluctuation-dissipation relation (FDR) $\frac{\partial\langle m\rangle}{\partial H} \equiv \chi_L^M = \frac{L^2\sigma_M^2}{T} \equiv \frac{X_L^M}{T}$ holds everywhere. Assuming H_c exists, is there a corresponding FDR between Q and H_c?

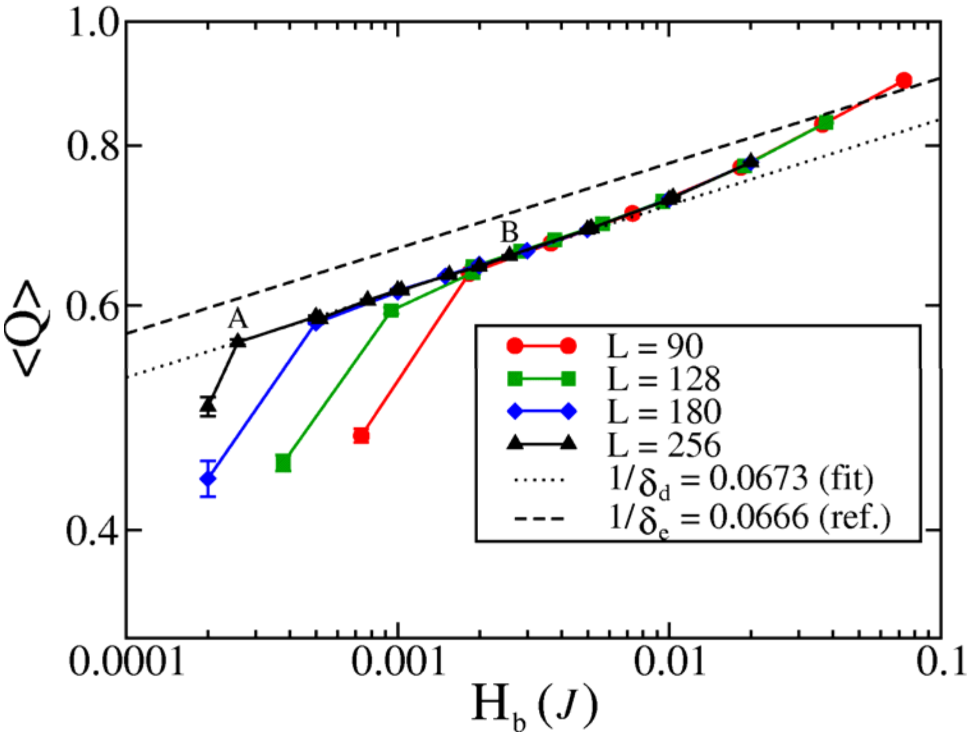
A: Yes, in the critical region (above $P = P_c$), for H_c not too large, an FDR between Q and H_c holds to a very good approximation.

D. T. Robb et al., Phys. Rev. E **76**, 021124 (2007)

Definition of H_b, direct scaling at $P = P_c$

$$H_b = \int_{t=iP}^{t=(i+1)P} H(t)dt$$

defines the period-averaged magnetic field, or 'bias field'



- **find power-law** $\langle Q \rangle \sim H_b^{1/\delta'}$ **at** $P = P_c$ **with** $\delta' = 14.85 \pm 0.18$
- **analogous to equilibrium scaling** $\langle m \rangle \sim H^{1/\delta}$ **at** $T = T_c$, **with** $\delta = 15$
- **note finite-size effects**

Predictions from finite-size scaling analysis

- **Treat finite-size effects in DPT systematically by writing scaling functions analogous to those used for equilibrium system**

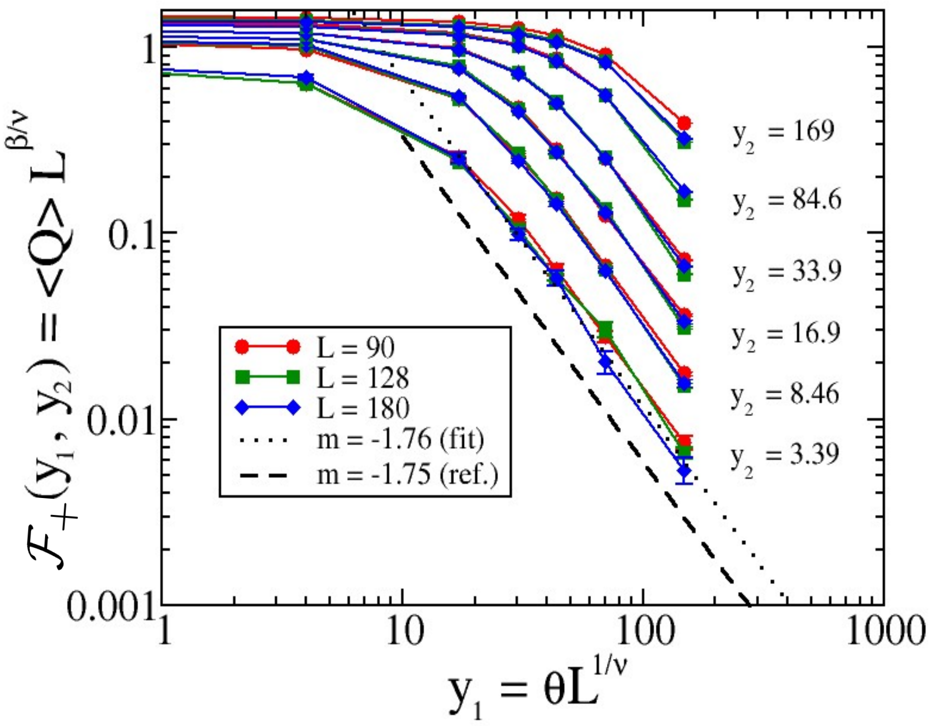
Scaling variables: $y_1 \equiv \theta L^{1/\nu} \equiv \left(\frac{P-P_c}{P_c}\right) L^{1/\nu}$ $\quad y_2 \equiv H_c L^{\beta\delta/\nu}$

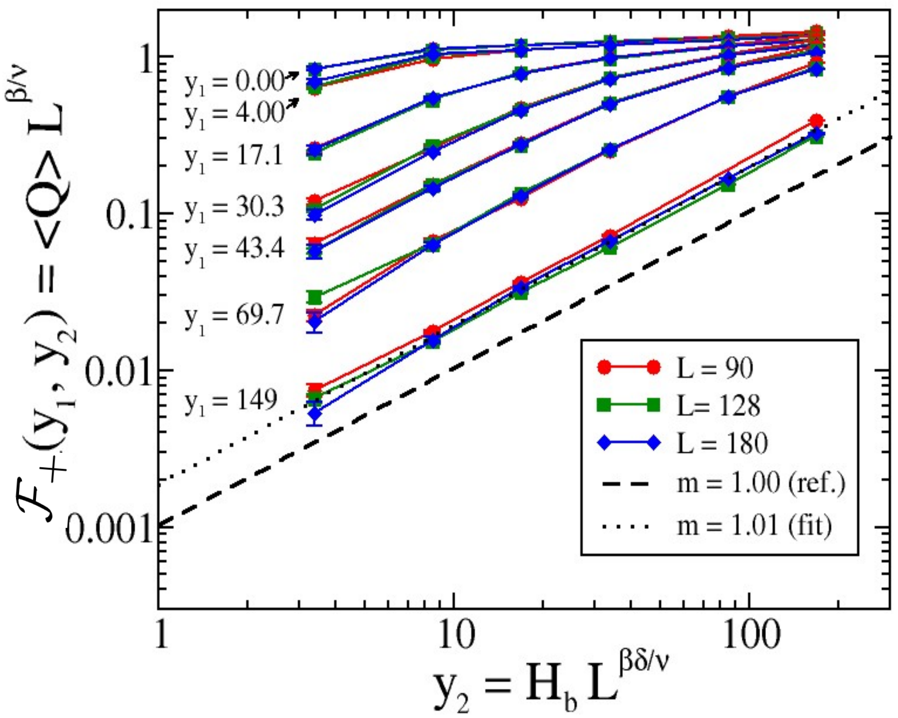
Scaling functions: $\mathcal{F}_+(y_1, y_2) \equiv \langle Q \rangle L^{\beta/\nu}$ $\quad \mathcal{G}_+(y_1, y_2) \equiv \hat{\chi}_L L^{-\gamma/\nu}$

- **Predicted asymptotic forms for scaling functions:**

$$\mathcal{F}_+(y_1, y_2) \sim \begin{cases} y_1^{-\gamma} y_2 & \text{for } y_1 \gg y_2 \\ y_2^{1/\delta} & \text{for } y_1 \ll y_2 \end{cases} \qquad \mathcal{G}_+(y_1, y_2) \sim \begin{cases} y_1^{-\gamma} & \text{for } y_1 \gg y_2 \\ y_2^{(1-\delta)/\delta} & \text{for } y_1 \ll y_2 \end{cases}$$

Numerical results for first scaling function ($\mathcal{F}_+$)





- **Find** $\mathcal{F}_+ \sim y_1^{-\gamma'}$ **with**

$\gamma' = -1.76 \pm 0.07$ **for** $y_1 \gg y_2$

- **Find** $\mathcal{F}_+ \sim y_2^{\omega'}$ **with**

$\omega' = 1.01 \pm 0.01$ **for** $y_1 \gg y_2$

Form of nonequilibrium FDR

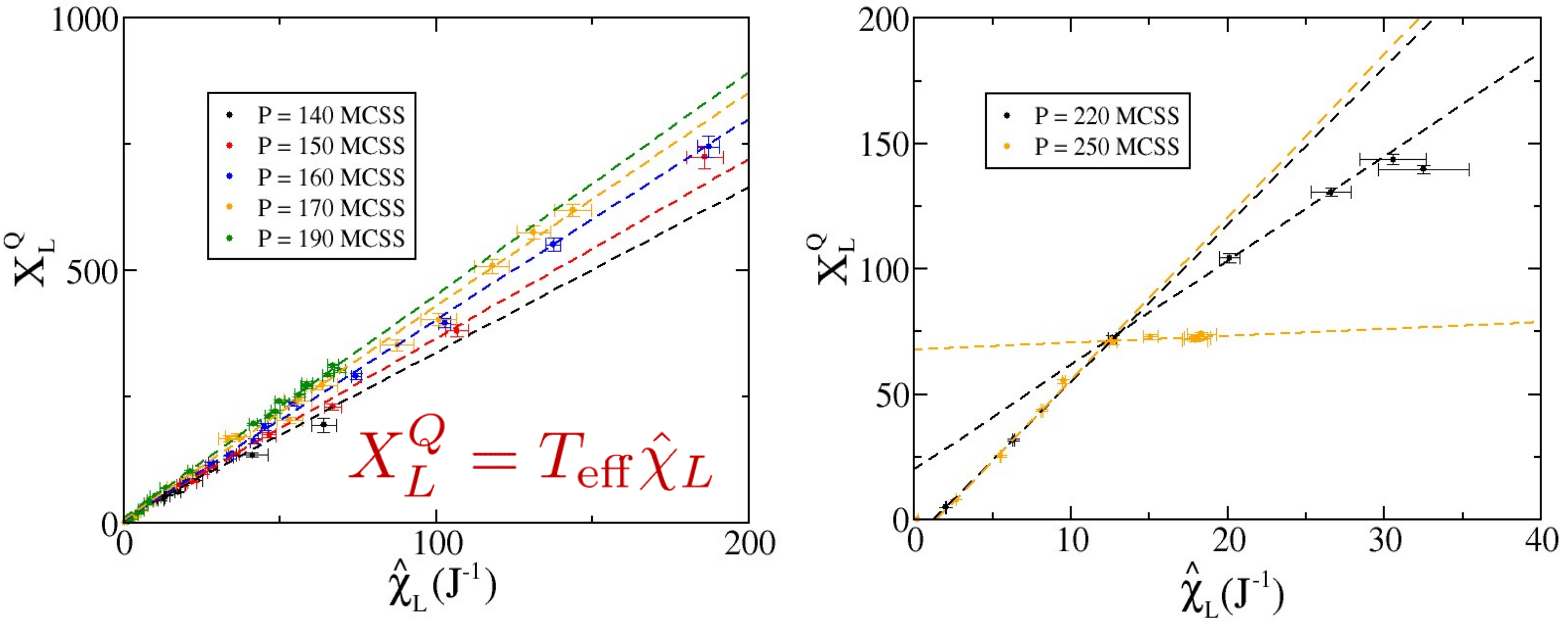
- **Equilibrium FDR:** $$\frac{\partial \langle m \rangle}{\partial H} \equiv \chi_L^M = \frac{L^2 \sigma_M^2}{T} \equiv \frac{X_L^M}{T}$$

  holds for all (*H*,*T*), since it follows directly from the partition function

- **Nonequilibrium FDR: does it hold?**

$$\frac{\partial \langle Q \rangle}{\partial H_b} \equiv \hat{\chi}_L \overset{?}{=} \frac{L^2 \sigma_Q^2}{T_{\text{eff}}} \equiv \frac{X_L^Q}{T_{\text{eff}}}$$

Numerical data on FDR

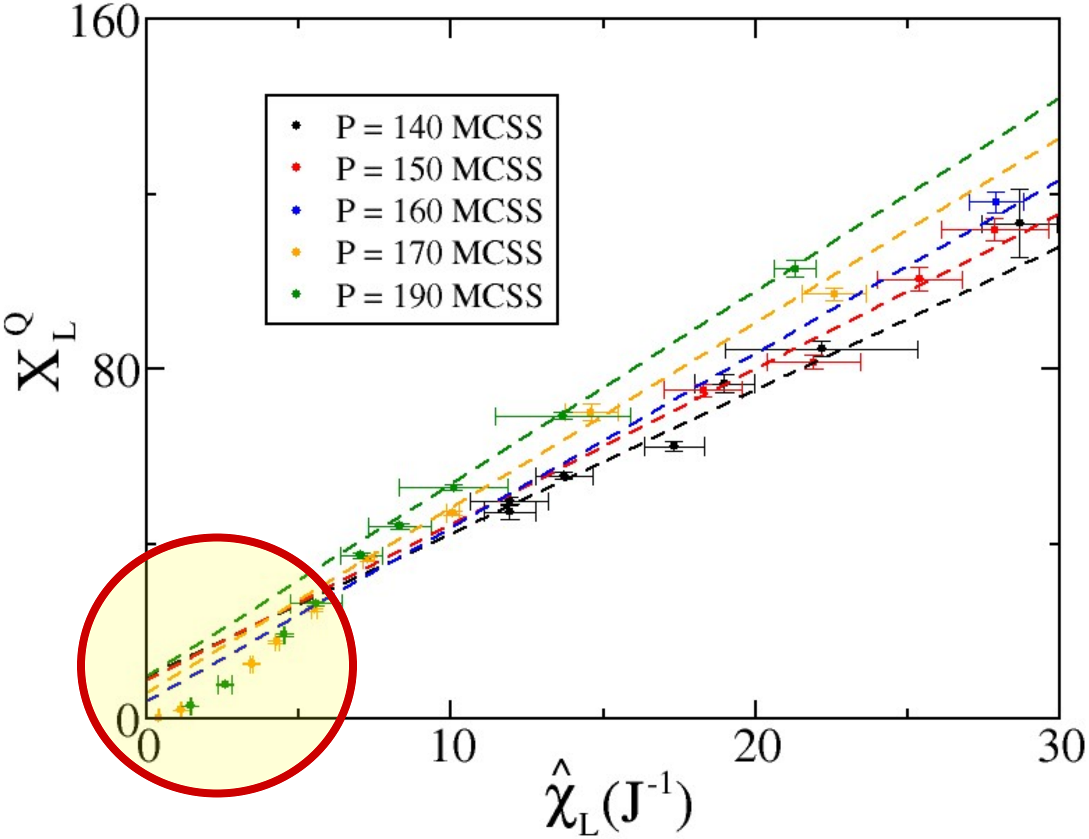


- **For** $P_c < P < 190$ **MCSS, find** $X_L^Q \sim \hat{\chi}_L$ **over wide range of** $\hat{\chi}_L$

  ($P_c = 136.96 \pm 0.75$**MCSS)**

- **For** $P \geq 220$ **MCSS, 'doubly linear' behavior → no unique** $T_{\rm eff}$

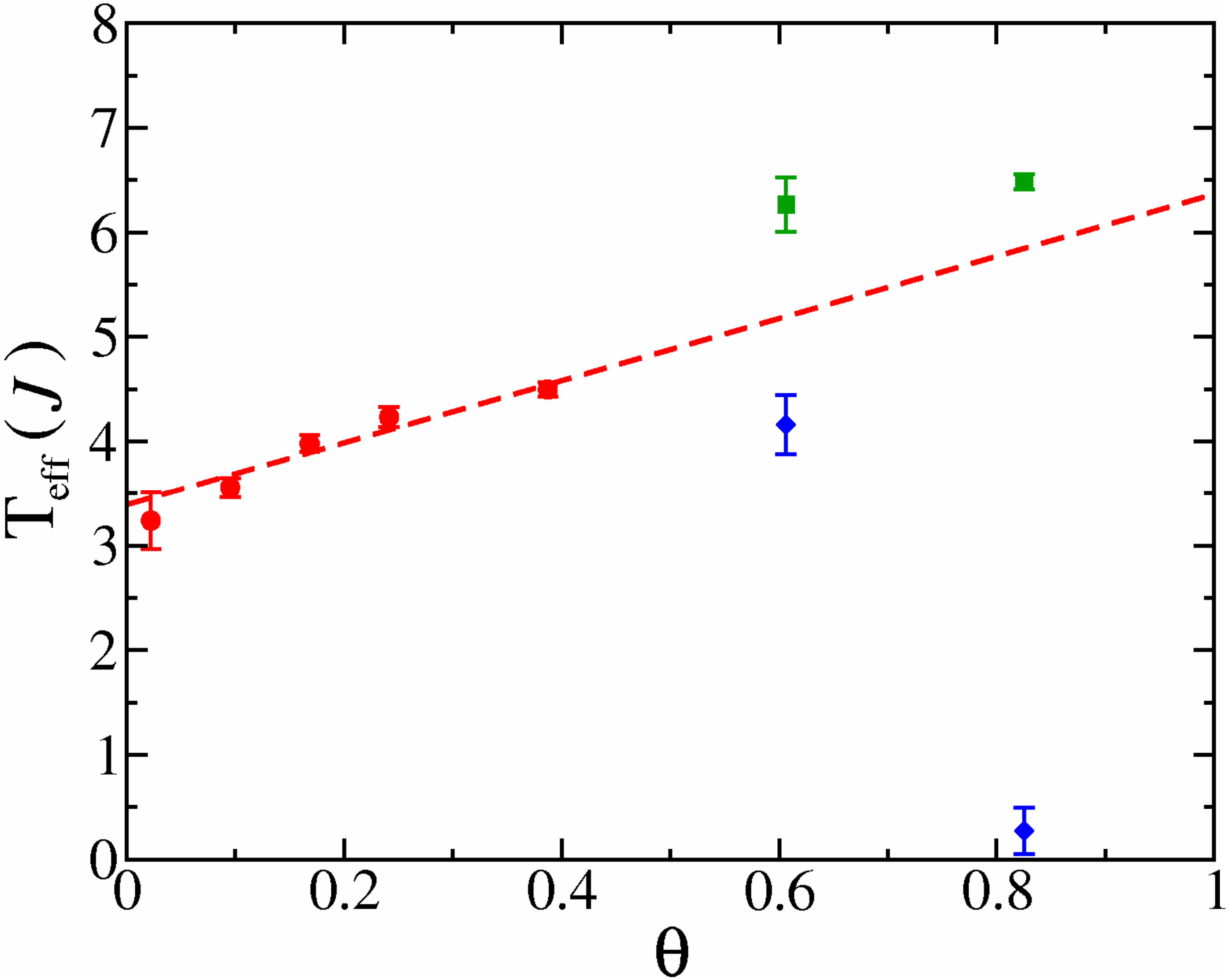
Numerical data on FDR: data at large H_b

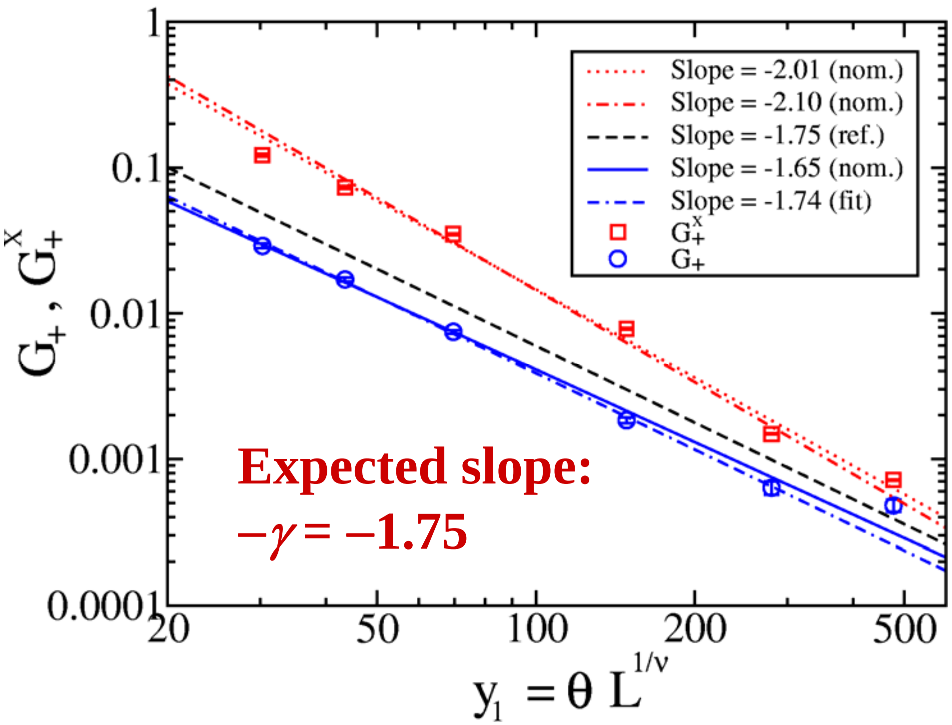


- **At low $\hat{\chi}_L$ values (large H_b values), relation $X_L^Q \sim \hat{\chi}_L$ breaks down**

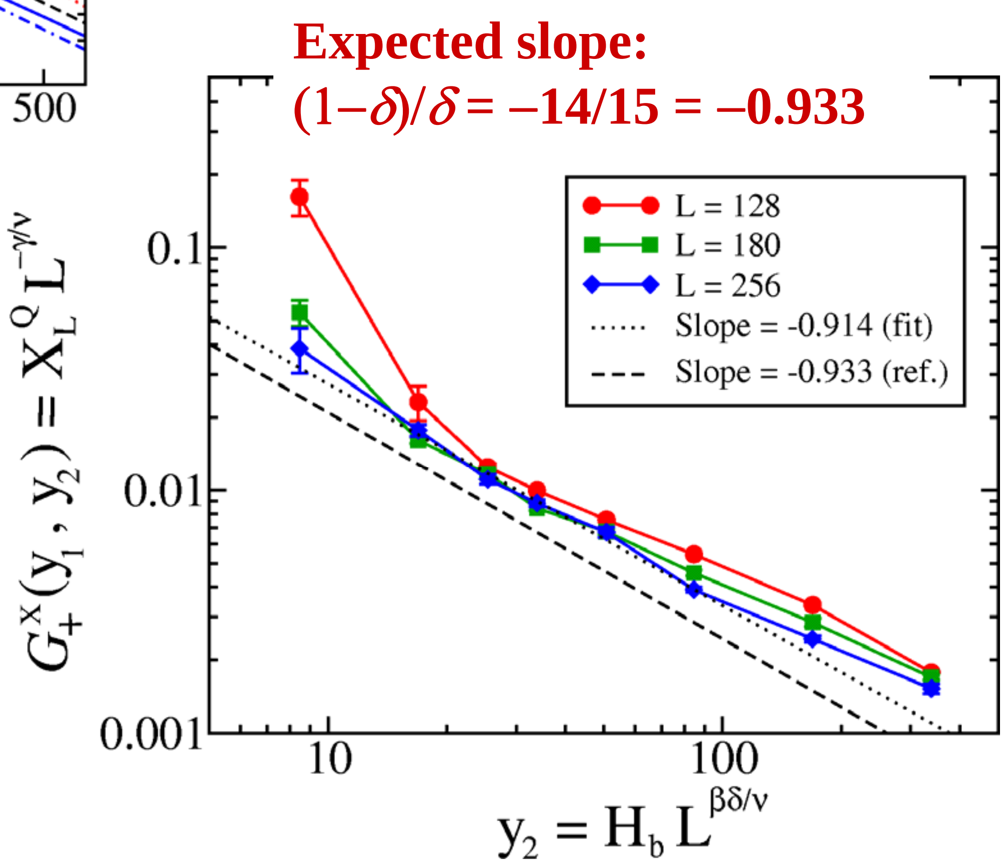
- **Use of X_L^Q as proxy for $\hat{\chi}_L$ in previous work (before H_b was identified) is still well- justified near $P = P_c$**

T_{eff} versus $\Theta = (P - P_c)/P_c$





Scaling functions $\mathcal{G}$
for susceptibility χ
and fluctuation X



Conclusions

- Hysteresis is a far-from-equibrium phenomenon found in many physical and chemical contexts, including magnetism, ferroelectrics, and surface adsorption
- Dynamic phase transition (DPT) for kinetic Ising model driven by oscillating field.
- Numerical and analytical evidence shows that the DPT at intermediate frequency is in the equilibrium Ising universality class
- Experimental evidence for DPT in Pt/Co multilayers
- Identified bias field as field conjugate to dynamic order parameter
- Numerically demonstrated nonequilribium Fluctuation-Dissipation relation in the critical region