# Phase Transitions & Scaling in QMC

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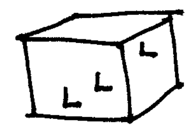
**Goal:** to characterize the properties of a thermodynamic phase transition using finite-size numerical simulations.

**Challenge:** no true phase transitions exist in a finite-size system: (finite size remnant only).

PBC



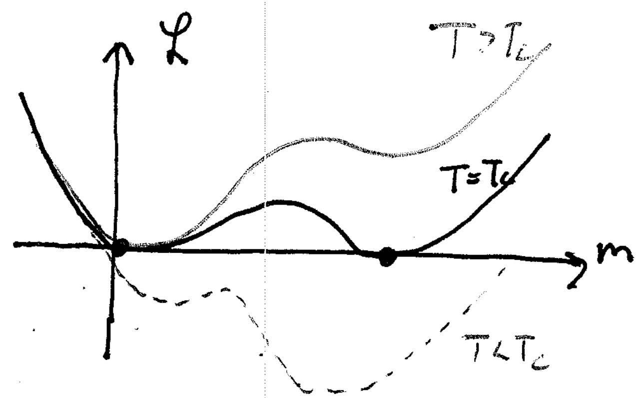

simulation cell.

**Solution:** use a combination of simulation data combined with Finite Size Scaling (FSS) theory.

**Phase transitions:** two important types to distinguish

1) first order: $\xi \to$ finite
2) continuous: $\xi \to \infty$

1) First-order transition

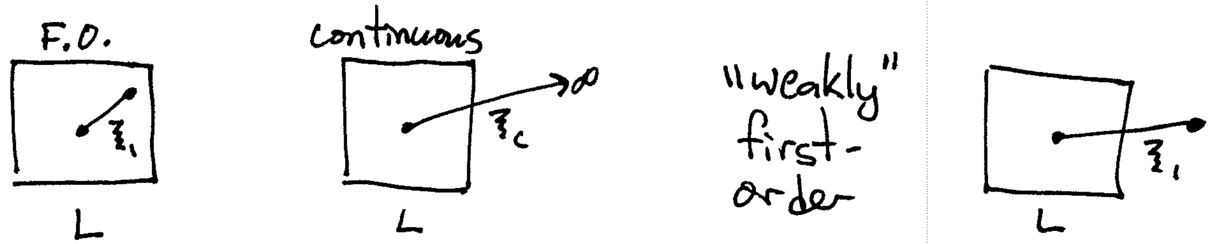



Recall Landau Free-energy density:

$$\mathcal{L} = a t m^2 + \tfrac{1}{2} b m^4 + c m^3$$

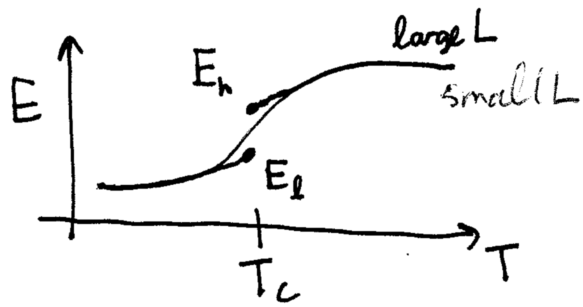
$$t = \frac{T-T_c}{T_c} \left( \text{or } \frac{h-h_c}{h_c} \right)$$

<u>Challenge</u>: distinguishing first-order from continuous phase transition on finite $L$:



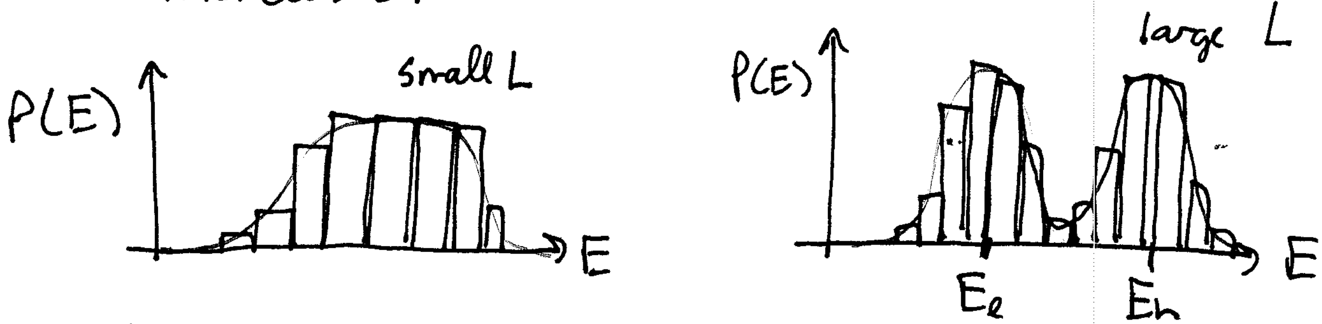

<u>Solution</u>: A series of criteria can be examined for signatures of F.O. behavior.

- A discontinuity develops in the (internal) energy as $L$ increases:




at $T_c$
- two-phase coexistence
- Latent heat is released.

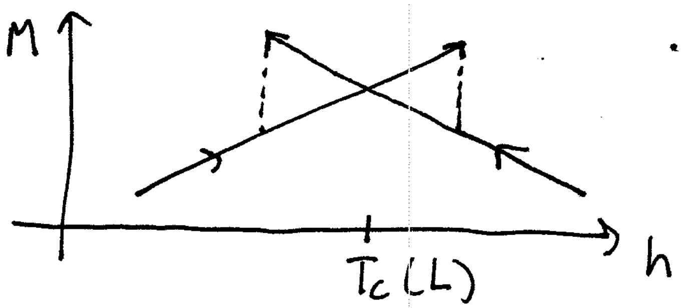
- Two-phase coexistence can be seen: the probability distribution of the internal energy develops a <u>double</u> peak as $L$ increases.




(also can be seen in magnetization, order p.)

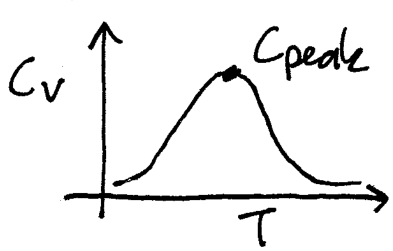
- Hysteresis: Monte Carlo simulations can become "stuck" in one of the free-energy minima, even if it is not quite the groundstate.

e.g: Magnetization

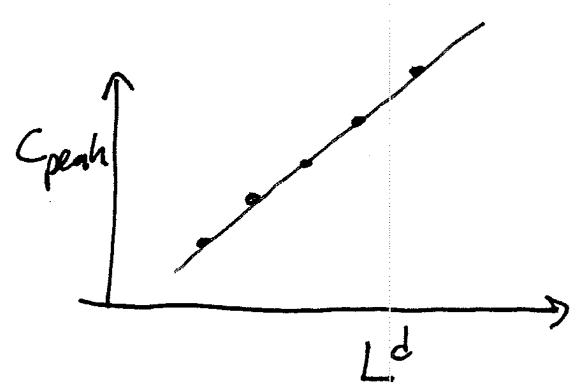



Metastability an indicator of "non-ergodicity" in a Monte Carlo simulation.

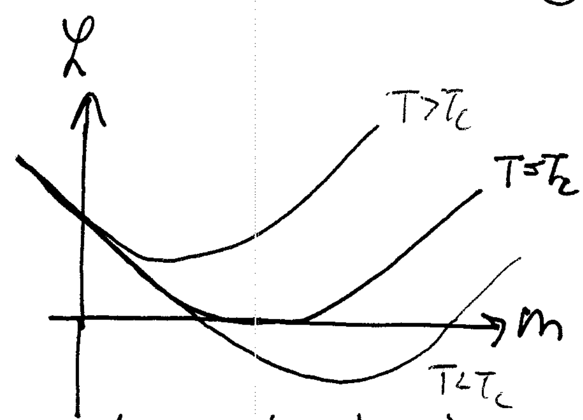
- Volume scaling of $C_V$, $\chi$ peaks
  - a result of $L$ being the only characteristic lengthscale.




$$C_{peak} = a + bL^d$$
$$\chi_{peak} = c + dL^d$$



## 2) Continuous transitions




Think of the Landau free-energy density

$$\mathcal{L} = atm^2 + \tfrac{1}{2}bm^4$$

(no cubic term)

(ie. no discontinuity etc. in E at $T_c$).

Most important consequence of $\xi \to \infty$:
universality & critical exponents, ie. critical exponents & other dimensionless properties are "universal". They only depend on
- symmetry of the underlying Hamiltonian
- dimension of system
- range of interaction.

Critical exponents calculated across various systems & techniques are identical for a given "universality class"
- field theory
- MC simulations
- experiments

Critical exponents: leading behavior of scaling of the divergence.

- Specific heat: $C_V \propto |t|^{-\alpha}$
- correlation length: $\xi \propto |t|^{-\nu}$
- susceptibility: $\chi \propto |t|^{-\gamma}$
- order parameter: $M \propto |t|^{\beta}$
- correlation function: $G(r) \sim r^{-(d-2+\eta)}$

anomolous dimension

(not all independent: recall "hyperscaling")

$$\alpha + 2\beta + \gamma = 2$$
$$\beta\gamma = \beta + \gamma$$
$$2 - \alpha = \nu d$$

→ Accurate values for universal critical exponents can be calculated in finite-size Monte Carlo simulations using finite-size scaling (FSS) theory:

Note that the correlation length "wants to" diverge as $\xi \propto |t|^{-\nu}$ but it is limited by the lattice size $L$:

$$\xi(T) = \left| \frac{T - T_c}{T_c} \right|^{-\nu} \quad (\text{where } T_c = T_c(\infty))$$

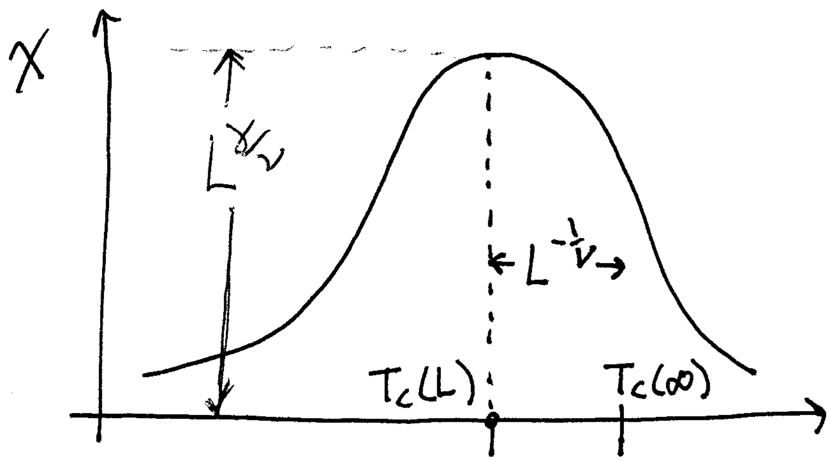
$$\xi(T)^{-\frac{1}{\nu}} = \left| \frac{T - T_c}{T_c} \right|$$

The role of $\xi$ is taken over by $L$

$$\left|\frac{T-T_c}{T_c}\right| \propto L^{-1/\nu}$$

at $T_c(L)$: $\quad T_c(L) - T_c(L=\infty) = aL^{-1/\nu}$

(i.e. a shift in the effective critical point)




Further, substitute $|t| \sim \xi^{-1/\nu} = L^{-1/\nu}$ in the expressions for the critical exponents:

if $\theta \propto |t|^{-x}$ in the temperature scaling law,
$\theta \propto L^{x/\nu}$ in the size-scaling law

More sophisticated: FSS theory derived from the ansatz:

$$\theta_L \sim L^{x/\nu} \mathcal{F}_\theta (tL^{1/\nu})$$

e.g.

$$M = L^{-\beta/\nu} \mathcal{F}_M (tL^{1/\nu}) \quad \text{etc.}$$

Exactly at the transition temperature, the scaling functions reduce to proportionality constants:

$$m \propto L^{-\beta/\nu}, \quad \chi \propto L^{\gamma/\nu}, \quad C_V \propto L^{\alpha/\nu}$$

- good data collapse corresponds to the correct $T_c$
- can be used to extract critical exponents

<u>Binder Cumulants</u>: magnetic moment ratios where non-universal scale factors cancel.

e.g. $$U_4 = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2}$$

for $L \to \infty$

$U_4 \to 0 \qquad T > T_c$

$U_4 \to U^* \qquad T = T_c$

$U_4 \to 2/3 \qquad T < T_c$

$U^*$ is universal. Is often very useful as a preliminary estimate for both $T_c$ and the universality class.

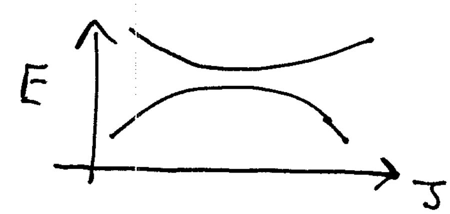
e.g. 2D Ising $\quad U^* = 0.610690(1)$

# Quantum Critical Scaling

$T=0$ transitions mediated by quantum fluctuations.
Define $t$ in analogy to reduced temperature

$$t = \left| \frac{J - J_c}{J_c} \right|$$

Continuous transition: avoided level crossing with a gap that closes $\Delta \sim |J - J_c|^{z\nu}$




We consider the formal mapping of the d-dimensional quantum problem to the d+1 dimensional effective classical problem with

$$L_\tau = \frac{\hbar}{k_B T} \quad \text{a "time" dimension}$$

The space and time directions are related by the dynamical scaling exponent $z$

$$\xi_\tau \sim \xi_r^z$$

(hence the finite-size gap scales as $L^{-z}$)

The most important change is that we replace the classical dimension $d$ with $d+z$ in the scaling relations

e.g.) hyperscaling: $\quad 2 - \alpha = \nu(d+z)$

e.g.) correlation function

$$G(r) \sim r^{-(d-2+\eta)} \rightarrow r^{-(d+z-2+\eta)} \text{ at QCP.}$$

note: $G(r) = \langle \sigma_i \sigma_j \rangle = \langle m^2 \rangle$ for $T < T_c$

in 2D: $\langle m^2 \rangle \sim L^{-(z+\eta)}$

also define $\chi_m = \frac{1}{N} \sum_{ij} e^{i \vec{r} \cdot \vec{q}} \int_0^\beta d\tau \langle S_i^z(\tau) S_j^z(0) \rangle$

$$\chi_m \sim L^{-\eta}$$

so $\langle m^2 \rangle$ and $\chi_m$ can be used to extract $z$ and $\eta$.

## Uniform susceptibility and spin stiffness

Stiffness: $\rho_s = \frac{\partial^2 F}{\partial \phi^2} = \frac{\langle W^2 \rangle}{\beta}$ $\qquad \beta = \frac{1}{T}$

Susceptibility: $\chi_u = \frac{\beta}{N} \langle (M^z)^2 \rangle$, $M^z = \sum_{i=1}^{N} S_i^z$

Two important additional FSS relationships are: (Chubukov, Sachdev, Ye, Fisher

$$\rho_s(T,L,J) = \frac{T}{L^{d-2}} \mathcal{F}_{\rho_s}\left(\frac{L^z T}{c}, tL^{1/\nu}\right)$$

$$\chi_u(T,L,J) = \frac{1}{TL^d} \mathcal{F}_{\chi_u}\left(\frac{L^z T}{c}, tL^{1/\nu}\right)$$

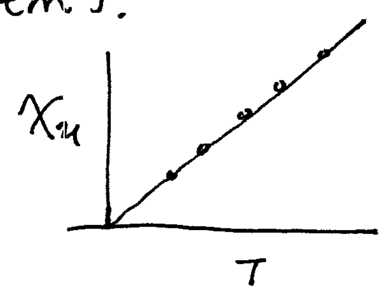
$\Rightarrow$ At criticality $(t=0)$

## $L \to \infty$ Uniform susceptibility

$$\mathcal{F}_{\chi_u}(x \to \infty, 0) = A_\chi \, x^{d/z} \qquad (A_\chi = \text{universal amplitude})$$

$$\chi_u \propto T^{(d/z - 1)}$$

e.g. $\chi_u$ should be $T$-linear for a $z=1$ transition, and should intercept the axis at $T=0$, (in a 2D system).

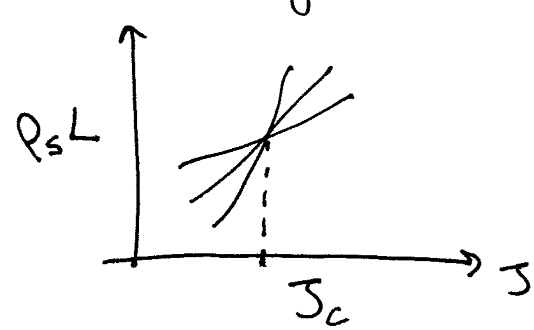



## $T \to 0$ spin stiffness

$$\mathcal{F}_{\rho_s}(x \to 0, 0) = A_\rho / x \qquad (A_\rho = \text{universal amplitude})$$

$$\rho_s \sim L^{2-d-z}$$

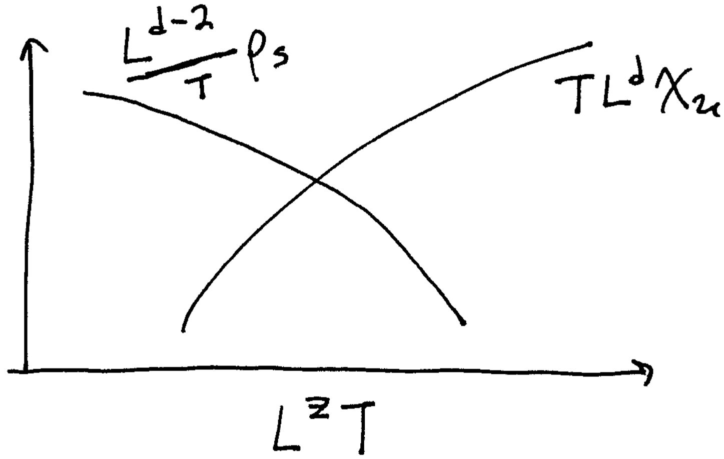
If $z=1$, in 2D the spin stiffness should have a crossing, if plotted as




$\leftarrow$ good estimate for $J_c$

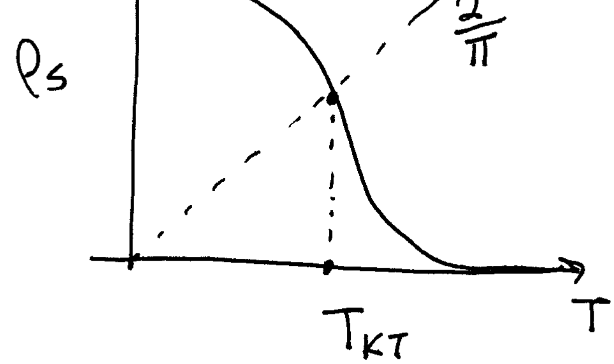
If $J_c$ is known, we can hold the second argument of the functions constant (tune to $t=0$): should then get data collapse to universal scale functions:

(in 2D)




## Kosterlitz - Thouless transitions

A special form of FSS analysis can be used in the vortex-unbinding transition in 2D superfluids:




Nelson-Kosterlitz "Universal Jump" condition:

$$\rho_s = \frac{2}{\pi} T_{KT}$$

A special FSS form can be derived from the Kosterlitz RG equations

$$\rho_s(L) = \rho_s(\infty)\left[1 + \frac{1}{2\ln(L) + C}\right]$$

as $T \to T_{KT}^-$

ie. $T_{KT}$ can be found by a $\chi^2$ goodness of fit to the straight-line form

$$Y(L) = \pi \ln(L) + C', \quad Y(L) = \left[\frac{\rho_s(L)}{T} - \frac{2}{\pi}\right]^{-1}$$

Alternatively, form the RG equations, as $T \to T_{KT}$

$$\xi \simeq e^{(bt^{-1/2})}$$

$b$ is some constant

if the correlation length is limited, $\xi = L/L_0$

$$T_{KT}(L) = T_{KT}(\infty)\left[1 + \frac{b^2}{\ln^2(L/L_0)}\right]$$