## Critical behavior and scaling

Correlation length $\xi$ defined in terms of correlation function

$$
C\left(\vec{r}_{i j}\right)=\left\langle\sigma_{i} \sigma_{j}\right\rangle-\left\langle\sigma_{i}\right\rangle^{2} \sim \mathrm{e}^{-r_{i j} / \xi}, \quad \vec{r}_{i j} \equiv\left|\vec{r}_{i}-\vec{r}_{j}\right|
$$

The correlation length diverges at the critical point

$$
\xi \sim t^{-\nu}, \quad t=\frac{\left|T-T_{c}\right|}{T_{c}} \quad \text { (reduced temperature) }
$$

$v$ is an example of a critical exponent

## Universality

Critical exponents do not depend on microscopic details of the interactions; only on the dimensionality of the system and the order parameter:

- Ising, gas/liquid (scalar Z2-symmetric order parameter)
- XY spins, phase of superconductor (2D, O(2) order parameter)
- Heisenberg spins (3D, O(3) order parameter)

Phase transitions fall into universality classes characterized by different sets of critical exponents

## Other critical exponents

Order parameter for $\mathrm{T}<\mathrm{Tc}$ (e.g., magnetization)

$$
\langle m\rangle \sim\left(T_{c}-T\right)^{\beta}
$$

In practice, calculate $\langle | m\left\rangle,\left\langle m^{2}\right\rangle\right.$
Susceptibility corresponding to order

$$
\chi=\frac{1}{N} \frac{1}{T}\left(\left\langle M^{2}\right\rangle-\langle | M| \rangle^{2}\right)
$$



Diverges at the critical point

$$
\chi \sim t^{-\gamma}
$$

Specific heat $\quad C=\frac{1}{N} \frac{1}{T^{2}}\left(\left\langle E^{2}\right\rangle-\langle E\rangle^{2}\right)$
Singular at Tc

$$
C \sim t^{-\alpha}
$$

The exponent $\alpha$ can be positive or negative (no divergence If negative; 0 can correspond to log divergence)

Magnetization of 2D Ising ferromagnet $\langle | m\left\rangle \sim\left(T_{c}-T\right)^{\beta}, \quad\left(T<T_{c}\right) \quad\right.$ for infinite system


Magnetization squared $\left\langle m^{2}\right\rangle \sim\left(T_{c}-T\right)^{2 \beta}, \quad\left(T<T_{c}\right)$


The exponent $\beta$ can be extracted for large L

Comparison with known 2D Ising model exponent

$$
\beta=1 / 8
$$




If Tc is not known, use it as an adjustable parameter and look for power-law behavior

## Finite-size scaling

For a system of length $L$, the correlation length $\xi \leq L$
Express divergent quantities in terms of correlation length, e.g.,

$$
\xi \sim t^{-\nu}, \quad \chi \sim t^{-\gamma} \sim \xi^{\gamma / \nu}
$$

The largest value is obtained by substituting $\xi \rightarrow L$

$$
\chi_{\max } \sim L^{\gamma / \nu}
$$

At what T does the maximum occur?

$$
\xi=a t^{-\nu}=L \Rightarrow t \sim L^{-1 / \nu}
$$

The peak position of a divergent quantity can be taken as Tc for finite L (different quantities will give different Tc )
$\gamma, \nu$ can be extracted by studying peaks in $\xi(T)$
Similarly for specific heat;

$$
C_{\max } \sim L^{\alpha / \nu}
$$

Susceptibility: $\quad \chi=\frac{1}{N} \frac{1}{T}\left(\left\langle M^{2}\right\rangle-\langle | M| \rangle^{2}\right)$


Diverges at the transition: $\quad \chi \sim\left|T-T_{c}\right|^{-\gamma}$

On a logarithmic scale


Specific heat

(actually $\alpha=0$ and log divergence for 2D Ising)

2D Ising model; $\gamma=7 / 4, \quad \nu=1$

$$
T_{c}=2 / \ln (1+\sqrt{2}) \approx 2.2692
$$



In general; find Tc and exponents so that large-L curves scale

Binder ratio $\quad Q=\frac{\left\langle m^{2}\right\rangle}{\langle | m| \rangle^{2}} \quad\left(Q_{2 n}=\frac{\left\langle m^{2 n}\right\rangle}{\left\langle m^{n}\right\rangle^{2}}, n=1,2, \ldots\right)$
Useful dimensionless quantity for accurately locating Tc Infinite-size behavior:

$$
\begin{aligned}
& \langle | m\left\rangle \sim t^{\beta}\right. \\
& \left\langle m^{2}\right\rangle \sim t^{2 \beta}
\end{aligned}
$$

Implies finite-size scaling forms

$$
\begin{aligned}
& \left\langle m^{2}\right\rangle \sim L^{-2 \beta / \nu} \\
& \langle | m\left\rangle \sim L^{-\beta / \nu}\right.
\end{aligned}
$$

Hence Q should be size-independent at the critical point

$$
Q \rightarrow 1 \text { for } T \rightarrow 0, \quad Q \rightarrow \text { constant for } T \rightarrow \infty
$$

$\mathrm{Q}(\mathrm{L})$ curves for different L cross at Tc ; often small corrections

Binder ratio: $Q=\frac{\left\langle m^{2}\right\rangle}{\langle | m| \rangle^{2}}$


Q is size independent at Tc (useful for locating Tc )


Scaling theory with corrections predicts:

$$
T^{*}(L, 2 L)=T_{c}+a L^{-(1 / \nu+\omega)}
$$

$\omega$ is an exponent governing scaling corrections, $\omega=2$ for 2D Ising

Crossing points for, e.g., sizes $\mathrm{L}, 2 \mathrm{~L}$ can be extrapolated to infinite L to give an accurate value for Tc


## Autocorrelation functions

Value of some quantity at Monte Carlo step i: $Q_{i}$
The autocorrelation function measures how a quantity becomes statistically independent from its value at previous steps

$$
A_{Q}(\tau)=\frac{\left\langle Q_{i+\tau} Q_{i}\right\rangle-\left\langle Q_{i}\right\rangle^{2}}{\left\langle Q_{i}^{2}\right\rangle-\left\langle Q_{i}\right\rangle^{2}} \quad \text { (averaged over time i) }
$$

Asymptotical decay

$$
A_{Q}(\tau) \sim \mathrm{e}^{-\tau / \Theta}, \quad \Theta=\text { autocorrelation time }
$$

Integerated autocorrelation time

$$
\Theta_{\mathrm{int}}=\frac{1}{2}+\sum_{\tau=1}^{\infty} A_{Q}(\tau)
$$

Critical slowing down

$$
\Theta \rightarrow \infty \text { as } T \rightarrow T_{c}
$$

At a critical point for system of length L ; $\mathrm{Q}=$ order parameter
$\Theta \sim L^{z}, \quad z=$ dynamic exponent

## General finite-size scaling hypothesis

The ratio $\xi / L=t^{-\nu} L^{-1}$ should control the behavior of finite-size data also close to Tc
Test this finite-size scaling form

$$
\chi(t)=L^{\sigma} f(\xi / L)=L^{\sigma} f\left(t^{-\nu} L^{-1}\right)=L^{\sigma} g\left(t L^{1 / \nu}\right)
$$

What is the exponent $\sigma$ ?
We know that for fixed (small) t , the infinite L form should be

$$
\chi(t) \sim t^{-\gamma}, \quad(L \rightarrow \infty)
$$

To reproduce this, the scaling function $g(x)$ must have the limit

$$
g(x) \rightarrow x^{b}, \quad(x \rightarrow \infty)
$$

We can determine the exponents as follows

$$
\chi(t) \sim L^{\sigma} g\left(t L^{1 / \nu}\right)=L^{\sigma}\left(t L^{1 / \nu}\right)^{b}=t^{b} L^{\sigma+b / \nu}
$$

Hence $b=-\gamma, \sigma=\gamma / \nu$

$$
\chi(t)=L^{\gamma / \nu} g\left(t L^{1 / \nu}\right)
$$

Find $g$ by graphing $\chi(t) / L^{\gamma / \nu}$ versus $t L^{1 / \nu}$

2D Ising autocorrelation functions for $|\mathrm{M}|$


Exponentially decaying autocorrelation function

- convergent autocorrelation time as Lincreases


Autocorrelation time diverges with L

## Critical slowing down

Dynamic exponent Z: $\Theta, \Theta_{\text {int }} \sim L^{Z}$


For the Metropolis algorithm (Metropolis dynamics) $Z \approx 2.2$

How to calculate autocorrelation functions
If we want autocorrelations for up to K MC step separations, we need to store $K$ successive measurements of quantity Q
Store values in vector tobs [1:K]; first k steps to fill the vector. Then, shift values after each step, add latest measurement: vector contents after MC step n

| $\mathrm{Q}_{\mathrm{n}}$ | $\mathrm{Q}_{\mathrm{n}-1}$ | $\mathrm{Q}_{\mathrm{n}-2}$ | $\ldots$ |  | $\ldots$ | $\mathrm{Q}_{\mathrm{n}-\mathrm{K}+1}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |

vector contents after MC step $\mathrm{n}+1$

| $\mathrm{Q}_{\mathrm{n}+1}$ | $\mathrm{Q}_{\mathrm{n}}$ | $\mathrm{Q}_{\mathrm{n}-\mathrm{L}}$ | $\ldots$ |  | $\ldots$ | $\mathrm{Q}_{\mathrm{n}-\mathrm{K}+2}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |

Accumulate time-averaged correlation functions of Q (variable q )

```
for \(\mathrm{t}=2: \mathrm{k}\)
    tobs[t]=tobs[t-1]
end
tobs[1] =q
for \(t=0: k-1\)
    acorr[t]=acorr[t]+tobs[1]*tobs[1+t]
end
```

