Lecture 19

Important quantities in phase transitions are correlation functions of quantities in space

Eg $g(r)$ - if particle is at $r=0$, what is (relative) likelihood of seeing one at dist r away

We found we could write this as

$$\langle \rho(0)\rho(\vec{r})\rangle \quad \text{where} \quad \rho(\vec{r}) = \sum_{i=1}^{N} \delta(\vec{r}-\vec{r}_i)$$

In a lattice model, compute spin-spin correlation function - ↑ - likely to be ↑ nearby but how far?

Let $\delta s_i = s_i - \langle s_i \rangle$

$$C_{ij} = \langle \delta s_i \, \delta s_j \rangle = \langle s_i s_j \rangle - \langle s_i s_j \rangle$$

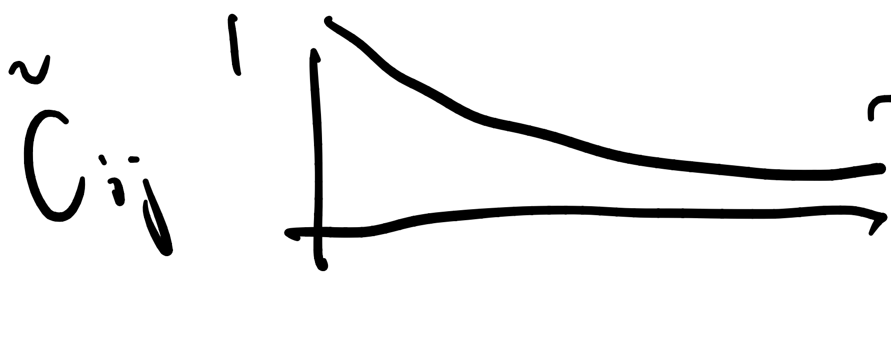
if i & j very far apart, could be independent

so then $\langle s_i s_j \rangle \to \langle s_i \rangle \langle s_j \rangle$

So $C_{ij} \to 0$ in this case

Note $C_{ii} = Var(s_i)$ so define

$$\tilde{C}_{ij} = C_{ij} / Var(s_i)$$



$\sim e^{-r/\xi}$

Volume ξ^d correlated

spins correlated w/ i $\approx \sum_{j \neq i} C_{ij}$

This is related to susceptibility in mag:

$$\chi = \frac{1}{N} \mathrm{Var}(\delta M) \qquad \delta M = \sum_{i=1}^{N} (s_i - \langle s_i \rangle)$$

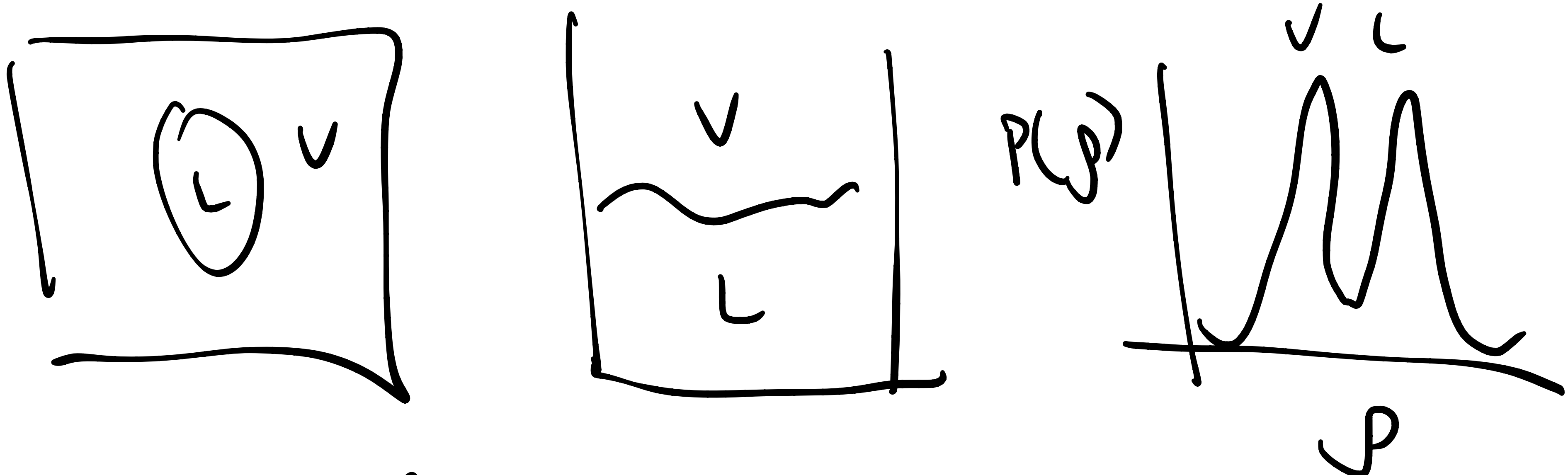
$$= \frac{1}{N} \sum_{ij} \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$$

$$= \frac{N}{N} \sum_{j} \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle = \sum_j C_{ij}$$

Since χ diverges at phase transition, means correlation volume grows

2 ways Var can diverge

1) 2 phase coexistence



as $N \to \infty$, P(ρ) gets sharp & var diverges

2) cts phase transition: no distinction,

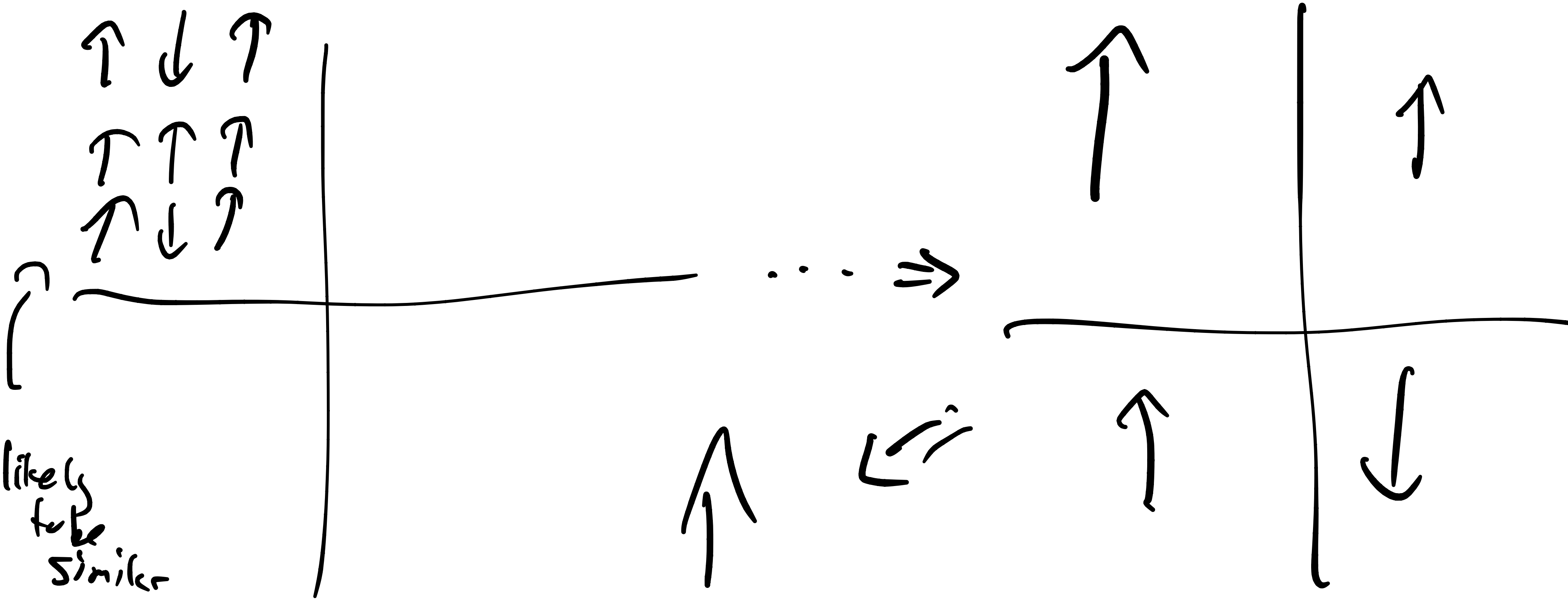
divergence means long range spatial correlations fit to $G(r) \sim C_{ij} \sim e^{-r/\xi} / r^{d-2+\eta}$

as $T \to T_c$ $\quad \xi \sim |T - T_c|^{-\nu}$

Large length scale <-> system looks similar on large & small length scales

Renormalization Group

coarse grain over part of system to get partition function that looks same



Eg block spin $\mathcal{H} = \sum_{\langle ij \rangle} J s_i s_j \to \sum_{\langle i',j' \rangle} J' s_{i'} s_{j'}$

Repeat: if $J \to J'$ process converges, then there is a fixed point, & this corresponds to a phase transition

From eqns that generate $J \to J'$,
can compute critical exponents!

For 2d ising, 0 field, find two stable
fixed points ($T=0$, $T=\infty$)
& 1 unstable fixed point

similar

$J/k_B T_c = 0.50648$ (Chandler Ch 5)

where exact is 0.44069

Book 261

iterations needed gets larger as closer to T_c,
connecting to a growing length scale

Intro to non-eq

So far we dealt with systems after they reach equilibrium

eg Heat flows in & out until $T_{bath} = T_{sys} = T$, doing work on the system

What happens during this process?

- time reversibility broken (at macro level)
- can reach non eq steady state w/ const driving but basically like eq

Eg: selfassembly by drying
in external field

molecular motors (ATP gradient)
folding/unfolding protein under force

Some theories for these real cases

<u>First</u> have to understand near-eq & dynamics
time dep processes

Brownian motion & Langevin eqn

Observation: pollen particles jiggle randomly

predictable behavior on average (Brown)

Einstein postulated, maybe due to random collisions w/ solvent

$$F_{total} = ma = m\frac{dv}{dt}$$

physical observations / Stokes - has drag

$$m\frac{dv}{dt} = -\xi v$$

$\xi = 6\pi \eta a$ viscosity, radius

for sphere