Monte Carlo Strategies for Spin Liquids

R. Melko

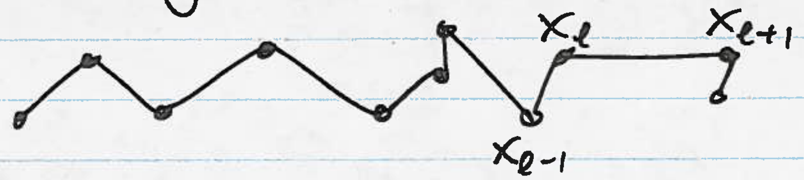
Lecture 1

- MC: probabilistic sampling of some classical d (or $d+1$) dimensional "configuration" x and calculation of observables.
- Spin liquids pose one of the biggest challenges to MC methods, which are widely used in other fields
- The sign problem (Monday's lecture) is a major bottleneck.

Goal of MCMC: calculate some expectation value (an equilibrium stat. mech. quantity)

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \mathrm{Tr}\{ e^{-\beta E} \mathcal{O} \} = \frac{\sum_x \mathcal{O}(x) W_x}{\sum_x W_x}$$

Sequence of configurations forms a Markov Chain



e.g.) $x_\ell = \uparrow\uparrow\uparrow\uparrow\uparrow$
$x_{\ell+1} = \uparrow\uparrow\uparrow\downarrow\uparrow$

Will not lay out the details of MCMC theory here - consult standard references.

Basic Metropolis algorithm:

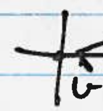
1. Choose an initial state x_1
2. Propose a trial change of state.
3. Calculate $\Delta E = E_{trial} - E_{old}$
4. If $\Delta E \leq 0$ <u>accept</u>: goto 7
5. If $\Delta E > 0$ calculate $p = e^{-\beta \Delta E}$
6. generate random $0 < r < 1$: accept if $r > p$
7. calculate estimators $\langle E \rangle$, $\langle M \rangle$ etc.
8. goto 2

Here, p has been determined via <u>detailed balance</u>:

$$W_x P(x \to y) = W_y P(y \to x)$$

Also, "Ergodicity" is a requirement. This depends on step 2: the proposed "trial" change.

Proceed with an example: 2D "<u>square ice</u>"

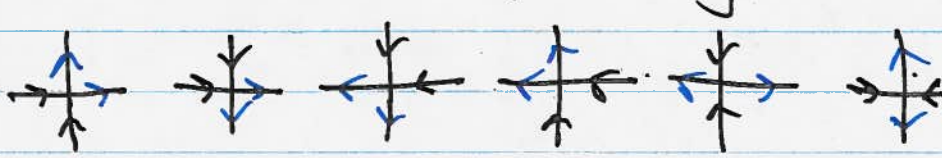
Ising D.O.F. on links:  "out"  "in" to vertex v

$$H = \sum_v Q_v^2, \quad Q_v = \sum_{i \in v} \sigma_i^z$$

$\sigma_i^z = 1$ <u>out</u>

$\sigma_i^z = -1$ <u>in</u>

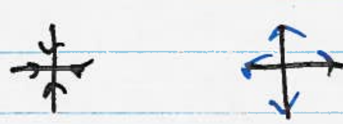
Produces a model where 6 of 16 vertices are energetically favored.



$E = 0$

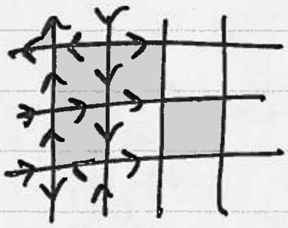
 ×4 and  ×4

$E = 4$



$E = 16$

<u>Groundstate</u>: extensively degenerate "manifold" of equal-energy states.



A type of classical spin liquid

Some properties:

- <u>Residual entropy</u>: Can be estimated in the pauling approximation from the "ice rules"
  1 – one σ^z D.O.F. per bond/link
  2 – two spins-in, two spins-out per vertex.

Rule 2: 6^{N_0} possible arrangements for N_0 vertices
Rule 1: Each bond has only a 50% chance of correctly satisfying both neighboring vertices

configurations: $6^{N_0}\left(\frac{1}{2}\right)^{N_1} = 6^{N_0}\left(\frac{1}{2}\right)^{2N_0} = \left(\frac{3}{2}\right)^{N_0}$

$\Rightarrow$ residual entropy (per vertex) $S = N_0 \log 3/2 = N_0\, 0.405$
(per spin) $S = N_1 \frac{1}{2} \log 3/2$

This is an approximation: the exact value due to Lieb is (per vertex) $S = N_0 \frac{3}{2} \log\left(\frac{4}{3}\right) \simeq N_0\, 0.432$

Can be calculated in <u>MC</u>: e.g. with the estimator
$$C = \frac{1}{T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right) \quad \text{(exercise)}$$

$C \equiv \frac{dE}{dT}$ & $dE = TdS$ $\Rightarrow$ $\Delta S = \int_{T_{low}}^{T_{high}} \frac{C}{T}\, dT$

$TdS = \frac{dE}{dT} dT$

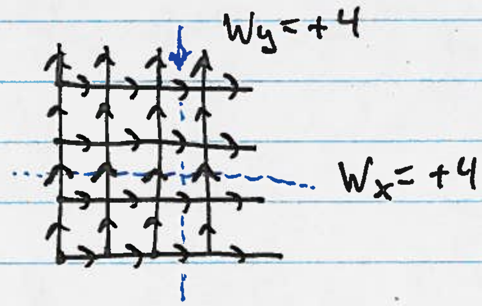
Thus, to calculate the groundstate <u>entropy</u>, a thermodynamic integration is required.

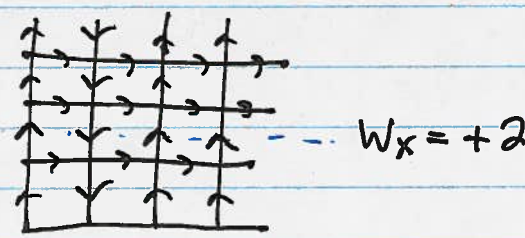
⇒ similar for <u>QMC calculations of topo EE</u>

- <u>Topological sectors</u>:

can be defined several ways (transition graph, vertex spins, height models).

e.g.)



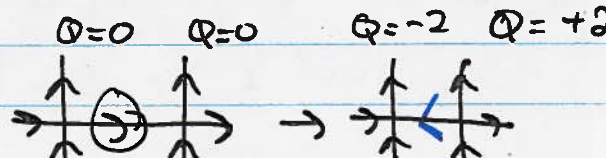


↑ flip whole line

This highlights an issue with <u>ergodicity</u>:

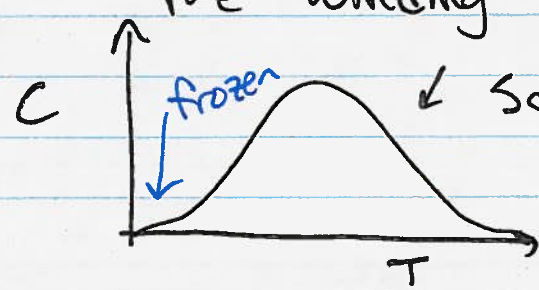
"the requirement that a Markov process be able to reach <u>any</u> state of the system from any other state."

Isolated single-spin flips



$\Delta E = 2 \cdot 4 - 0$

will be exponentially suppressed at low temperature, locking in the winding # sector.

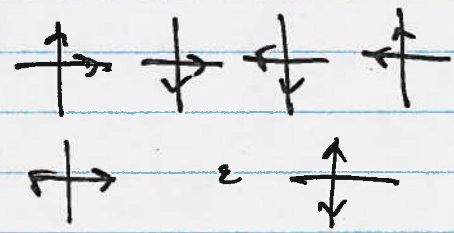


↙ Schottkey peak

Who cares if ergodicity is broken?

- any realistic classical system will have perturbations:

"F-ice"

e.g. 

$E = \varepsilon$

$E = 0$

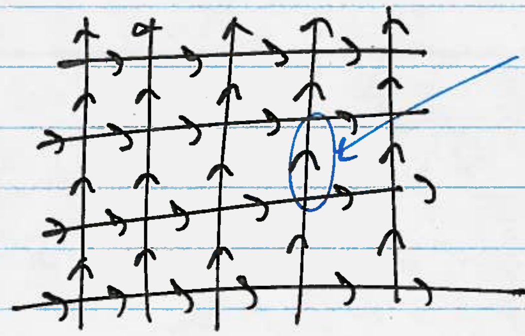
ε some small perturbation

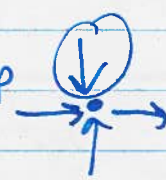
ie. a unique groundstate will be selected by ε: you may want to find it.

- topological properties (eg. winding #s) require non-local updates to sample.

<u>Non-local updates</u>: loops

no "defects"



- flip 

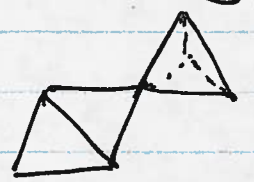
- choose one of the remaining 2 outgoing spins & repeat.

The loop is formed when the "head" meets the "tail". The energy change is evaluated & metropolis is used as usual on ΔE.

Single spin flips + loops required for ergodicity in this model.

Spin Ice:

3D analog of 2D square ice.

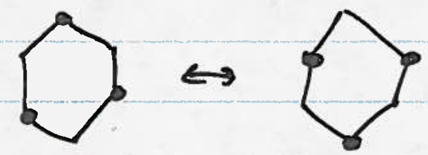


ice rules ⇒ 2 in - 2 out per tetrahedron.

Real materials, $Ho_2Ti_2O_7$ and $Dy_2Ti_2O_7$

$$H = \underbrace{-J \sum_{\langle ij \rangle} \vec{S}_i^{z_i} \cdot \vec{S}_j^{z_j}}_{\text{promotes spin-ice physics}} + \underbrace{\text{Dipolar interaction}}_{\text{selects unique groundstate.}} \left(\frac{1}{r^3}\right)$$

→ minimal loop: six spins



Spin ice is the prototypical success story
experiment ↔ M.C. simulation ↔ theory.

Quantum extensions - Q.S.I.

$$H \to H + (S^+S^- + S^-S^+) + (S^+S^+ + S^-S^-)$$

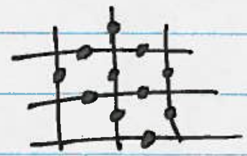
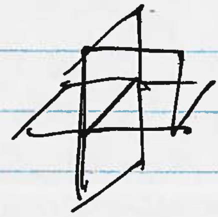
require Quantum Monte Carlo...

e.g. XXZ model shown to have U(1) lattice gauge theory by QMC ~~(Isakov,~~ (Banerjee, Isakov, Damle, Kim)

Classical $\mathbb{Z}_2$ gauge theories

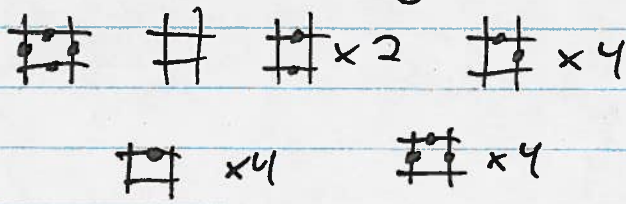
See e.g. Kogut Rev. Mod. Phys. 51, 659 (1979)

in $d \geq 2$ dimensions $\quad H = -\sum_p \prod_{i \in p} \sigma_i^z$

2d   3d

$$= -\sum_p \sigma_i^z \sigma_j^z \sigma_k^z \sigma_l^z$$

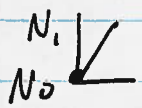
$\Rightarrow$ even number of $\sigma^z = 1$ around each plaquette.



$\rightarrow$ 8 vertex model $E = -1$

$\rightarrow$ $E = +1$ (excitation)

"Pauling" estimate for the residual entropy:



total D.O.F $= dN_0 = 2^{2N_0}$ configurations.

for every plaquette, $8/16$ will satisfy the $E=-1$ rules.

$$\Omega = \left(\tfrac{8}{16}\right)^{N_2} 2^{dN_0}$$

<u>or</u>: • There are 8 possible configurations per plaquette

• In 2D, each edge has a 50% chance of being satisfied.

2D

$\#$ configs: $\quad 8^{N_2}\left(\frac{1}{2}\right)^{N_1} = 8^{N_0}\left(\frac{1}{2}\right)^{2N_0} = (2)^{N_0}$

residual entropy (per vertex): $\quad S = N_0 \log 2$

Groundstate: degenerate manifold of equal-energy 8-vertex configurations. NO order parameter.

Finite-temperature phase transition?

- $d=2$ NO: Peierls argument.
- $d>2$ YES:

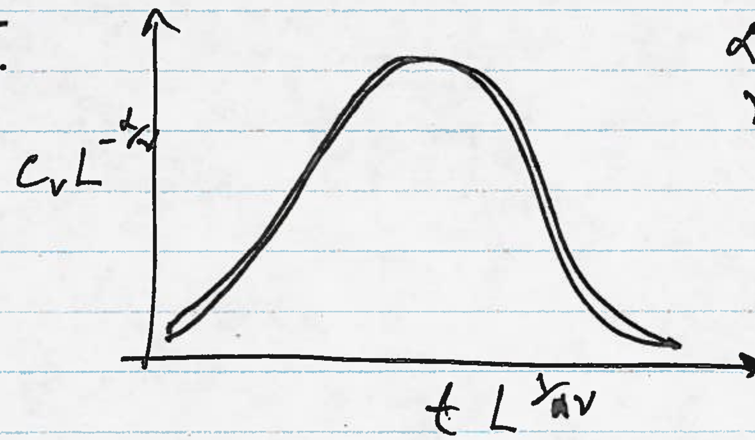
Monte Carlo can study the confinement / deconfinement (area-law to perimeter law) transition.

e.g. C_V versus T.

collapse to determine

$t = T - T_c$

3D: $\boxed{T_c = 1.313}$

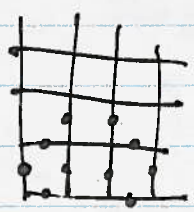


$\alpha = 0.110$
$\nu = 0.630$

Other properties of the low-temperature phase:

- stable topological winding number:

e.g. 2D



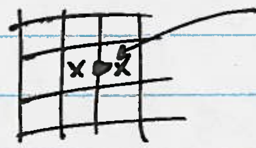
$(W_x, W_y) = (0,0)$
$(1,0)$
$(0,1)$
$(1,1)$

$\mathbb{Z}_2$ topological "order" (degeneracy)

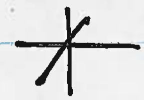
- Topological "entanglement" entropy ...

ON Monte Carlo sampling & ergodicity.

- local moves (SSF) are expected to be non-ergodic

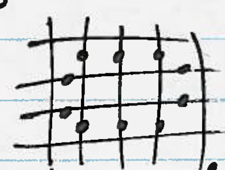


creates two ~~energy~~ "fractional" charges
but : finite energy barrier to creation.

- Non-local "gauge" flip: choose a vertex
  and flip all associated spins
   or  in 3d, etc.

  is ergodic within a winding # sector.

- Non-local "loop" moves



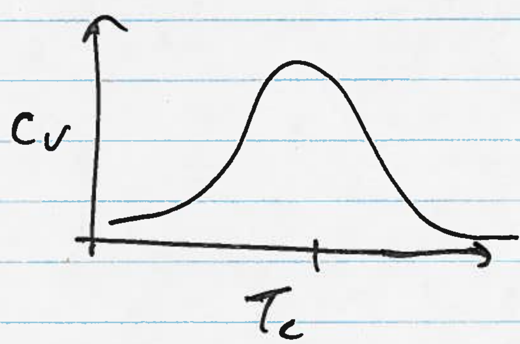
  samples winding # sectors provided loops are allowed to wind themselves.

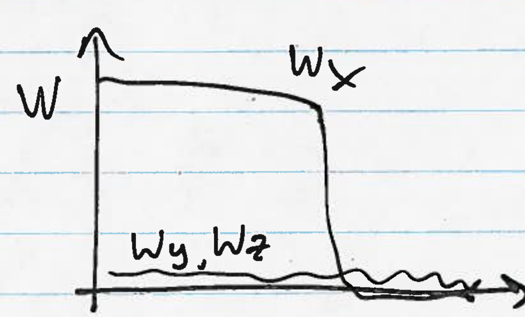
In all cases, ΔE should be calculated & a Metropolis' rejection/acceptance step performed.

Some signals of the transition will depend on the update:

e.g.

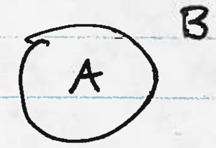
3d





Monte Carlo estimator for entropy of a "region"

Consider your Boltzmann probability:



$$p = \frac{1}{Z} e^{-\beta E} = \frac{1}{Z} e^{-\beta E(i_A, i_B)} = p_{i_A i_B}$$

Now trace out all the states of region B

$$p_{i_A} \equiv \frac{1}{Z} \sum_{i_B} p_{i_A i_B} = \frac{1}{Z} \sum_{i_B} e^{-\beta E(i_A, i_B)}$$

$$p_{i_A}^2 = \frac{1}{Z^2} \left(\sum_{i_B} e^{-\beta E(i_A i_B)} \right) \left(\sum_{j_B} e^{-\beta E(i_A j_B)} \right)$$

$$\mathrm{Tr}_A\, p_{i_A}^2 = \frac{1}{Z^2} \underbrace{\sum_{i_A} \sum_{i_B} \sum_{j_B} e^{-\beta \left[E(i_A, i_B) + E(i_A, j_B) \right]}}_{Z'[A,2,T]}$$

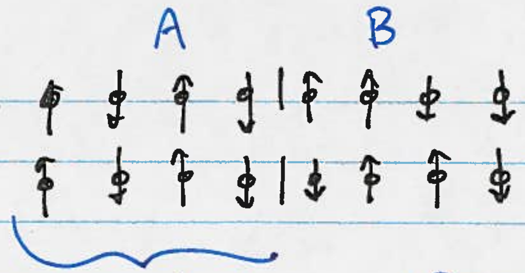
From the Renyi entropies $S_n = \frac{1}{1-n} \log(\mathrm{Tr}\, \rho_A^n)$

$$\Rightarrow S_2^{(A)} = -\log\left[Z'(A,2,T) \right] + 2 \log Z$$

Equivalent to the calculation of two free energies: one for the modified partition function $Z'[A,2,T]$, and the "regular" Z.

Monte Carlo: importance-sample from a probability distribution, generating configurations.

The partition function $Z'[A,2,T]$ is a special "replicated" simulation cell.

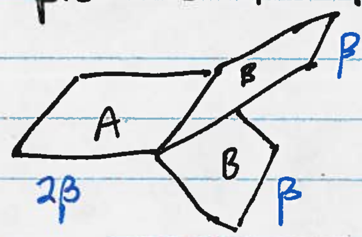


1D configuration

replica

constrained to be the same in region A.

Schematic picture in the continuum: a "Book"



- single copy of A at 2β
- two independent copies of B at β

A similar picture for $S_3, S_4, S_5 \cdots$ only <u>integer</u> Renyi indices possible for MC.

How to sample free-energies from these configurations?

- Thermodynamic integration:

$$S_2(A) = -S_A(\beta=0) + \int_0^\beta \langle E\rangle_A \, d\beta + 2S_0(\beta=0) - 2\int_0^\beta \langle E\rangle_0 \, d\beta$$

modified Z' (multi-sheeted) regular Z

- Direct ratio calculation: $\dfrac{Z'[A,2,T]}{Z^2}$

"acceptance ratio"
Bennett 1976
Roscilde 2012

Perform a MC move $Z^2 \leftrightarrow Z'$

$$\frac{Z'[A,2,T]}{Z^2} = \left\langle \frac{N_A}{N_{A=\emptyset}} \right\rangle_{MC}$$

M.C steps in a given region A, or $A=\emptyset$

What good is this classical entropy $S_n(A)$?

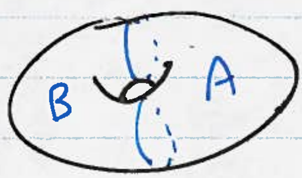
A finite-T, is extensive (in region A): highly non-universal.

Form the Mutual Information: $I_n(A;B)$

$$I_n(A;B) = S_n(A) + S_n(B) - S_n(A \cup B)$$

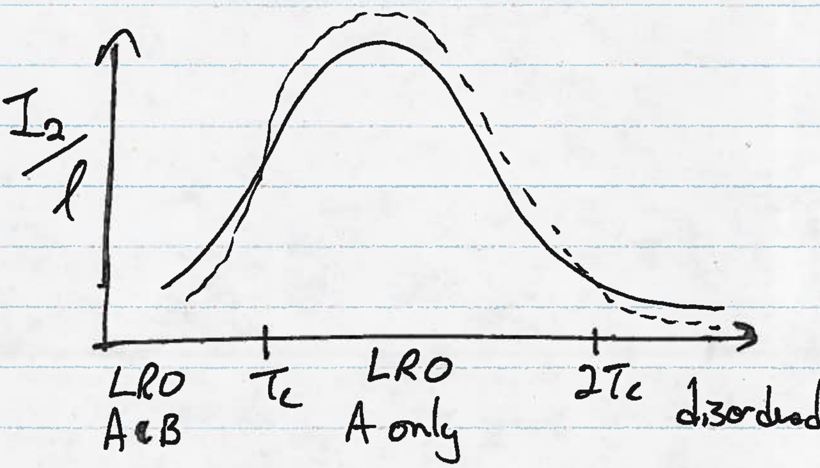
Gives leading-order area-law behavior by construction. Bounds correlation functions in a very precise way (Wolf, Verstraete, Hasting, Cirac, 2008 PRL)

e.g.) 2D Ising model



$L \times L$ torus.

Boundary $\ell = 2L$



$$I_2 = a(t)\,\ell + c(t) + O\left(\tfrac{1}{\ell}\right)$$

↑ changes sign through $2T_c$, T_c

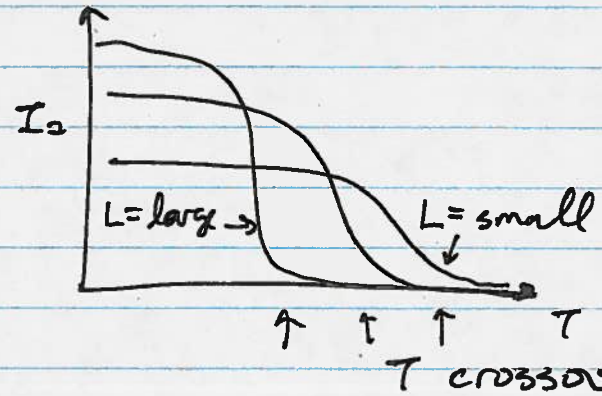
$c(t)$ generally depends on the shape of region A, can be used to determine universal properties of the critical theory (e.g. central charge).

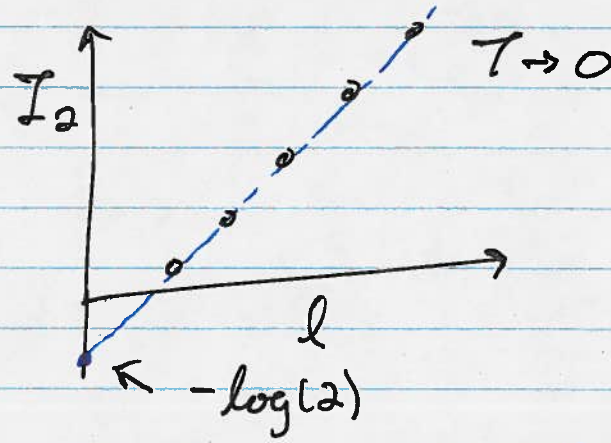
$$c(t) = \frac{c}{2}\,\frac{1}{n-1}\,f\left(\frac{L_A}{L}\right) \qquad \text{Stephan, J-M et. al.}$$

(No order parameter needed...)

Back to $\mathbb{Z}2$ gauge theories

2d.)





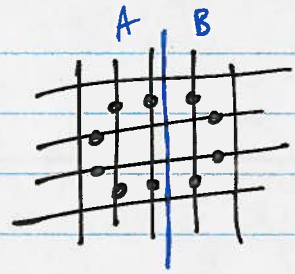
Crossover temperature?

energy of a defect.

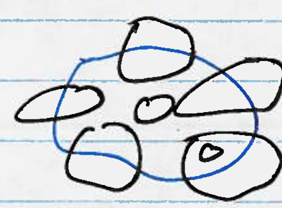
Probability of having a defect: $L^2 e^{-E_d/k_B T}$ reaches $\mathcal{O}(1)$, then topo EE decays

$$L^2 e^{-E/T} \sim 1 \Rightarrow T_{\text{crossover}} \propto \frac{E_d}{\log L}$$

T=0 intercept?



$\Rightarrow$



closed $\mathbb{Z}_2$ loop structure.

Intuition: what is the total number of accessible microstates for this boundary?

$$\Omega = 2^{l-1} \Rightarrow S \sim l \log 2 - \log 2 \sim a l - \log 2$$