

Title: PSI 2017/2018 - Machine Learning for Many Body Physics - Lecture 4

Date: Apr 12, 2018 09:00 AM

URL: <http://pirsa.org/18040057>

Abstract:

Outline for today:

- ↳ methods that prevent overfitting
- ↳ using supervised NNs to learn features of phases of matter
 - ↳ Ising model
 - ↳ Ising $\mathbb{Z}_2$ gauge theory

Methods that prevent overfitting

① L1 or L2 regularization

↳ adds an extra term to the cost function that depends on the magnitudes of the weights

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$$C = C_{\text{init}} + \frac{\lambda}{2D} \sum_{\text{weights}} (W_{ij}^{(l)})^2$$

Methods that prevent overfitting

① L1 or L2 regularization

L2 adds an extra term to the cost function that depends on the magnitudes of the weights

$$C = C_{\text{init}} + \frac{\lambda}{2D} \sum_{\text{weights}} (W_{ij}^{(l)})^2 \quad (\text{L2})$$

Ising $\mathbb{Z}_2$ gauge Theory

$$C = C_{\text{init}} + \frac{\lambda}{|\mathcal{D}|} \sum_{\text{weights}} |W_{ij}^{(e)}| \quad (L1)$$

$\lambda > 0$ is the regularization hyperparameter

Ising $\mathbb{Z}_2$ gauge Theory

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- λ too small

$$C = C_{\text{init}} + \frac{\lambda}{|\mathcal{D}|} \sum_{\text{weights}} |W_{ij}^{(e)}| \quad (L1)$$

$\lambda > 0$ is the regularization hyperparameter

- λ too small $\rightarrow$ overfitting
- λ too large $\rightarrow$ underfitting

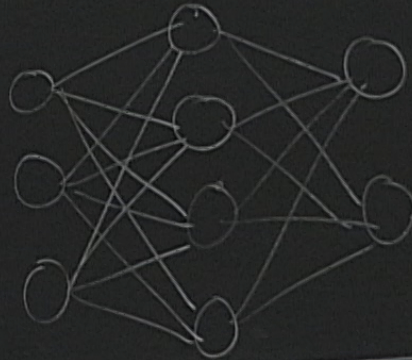
Effect: NN favours smaller weights

⇒ small change (added noise) to the training data will not have a large effect on the NN's behaviour

② Dropout

Randomly-selected neurons are temporarily masked out of the NN

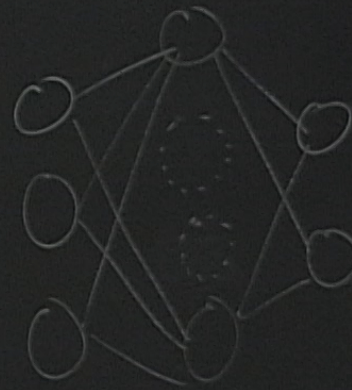
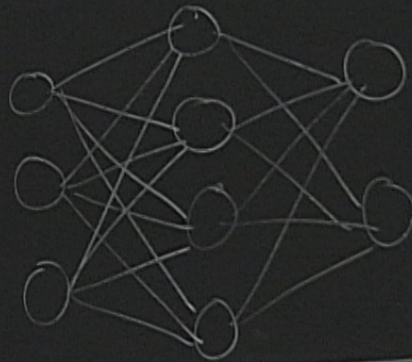
eg)



② Dropout

Randomly-selected neurons ^{in the hidden layer(s)} are temporarily masked out of the NN

eg)



- Run the training algorithm for some subset of data
- Choose a new random masking and repeat

Has a similar

- Run the training algorithm for some subset of data
- Choose a new random masking and repeat

Has a similar effect to averaging over many different NNs (each of which could overfit in different ways).



Distinguishing phases of matter using SL

↳ Carrasquilla & Melko, arXiv:1605.01735

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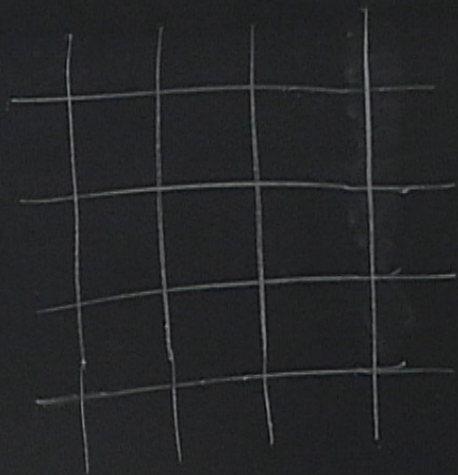
Classical Ising model

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i$$

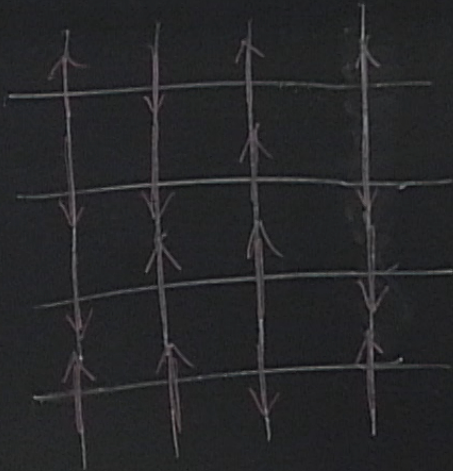
The d.o.f. σ_i are on
the sites of a lattice

$$\sigma_i = \begin{matrix} +1 & \text{or} & -1 \\ (\uparrow) & & (\downarrow) \end{matrix}$$

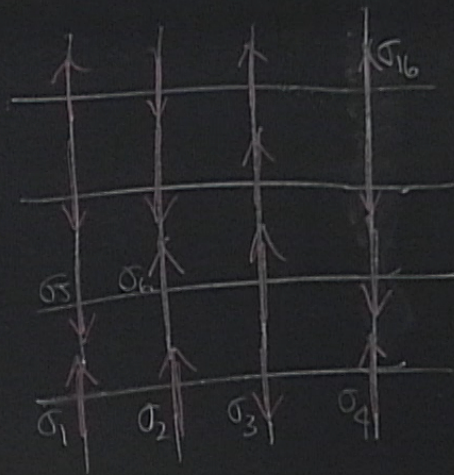
eg) 2D square lattice



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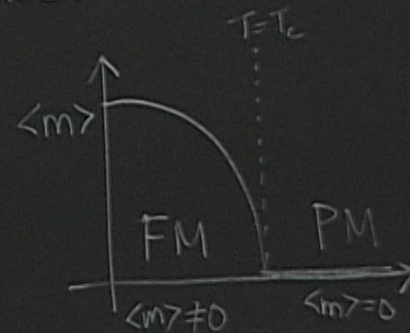
$L \times L$ lattice

$L=4$

On a 2D square lattice, we know that there is a phase transition from a ferromagnetic (FM)

to a paramagnetic (PM) phase. When $h=0$: $T_c \cong 2.269J$

In the thermodynamic limit:



order parameter:

$$\langle m \rangle = \frac{1}{N} \sum_i \sigma_i$$

Goal: train a NN to learn how
to classify the FM and PM labels
(Homework #1)

$$\approx 2.269 J$$

order parameter:

$$\langle m \rangle = \frac{1}{N} \sum_i \sigma_i$$

Input data: spin configurations

$$\vec{X} = [+1, +1, -1, +1, -1, \dots, +1]$$

$\uparrow \quad \uparrow \quad \quad \uparrow$
 $\sigma_1 \quad \sigma_2 \quad \quad \sigma_N$

Labels: $y=0$ or 1
 $\uparrow \quad \uparrow$
FM PM

U_s

Use Monte Carlo (MC) to generate the spin configuration samples
(we will discuss MC methods tomorrow)

FM

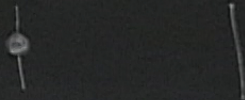
PM

Classical Ising gauge theory

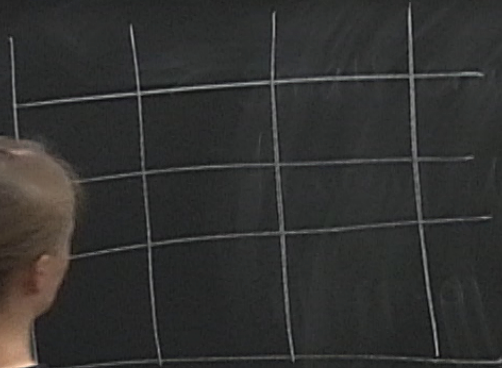
$$H = -J \sum_{\text{plaquettes } p} \left(\prod_{i \in p} \sigma_i \right)$$

The d.o.f. are on the bonds of the lattice

$$\sigma_i = +1 \quad \text{or} \quad -1$$

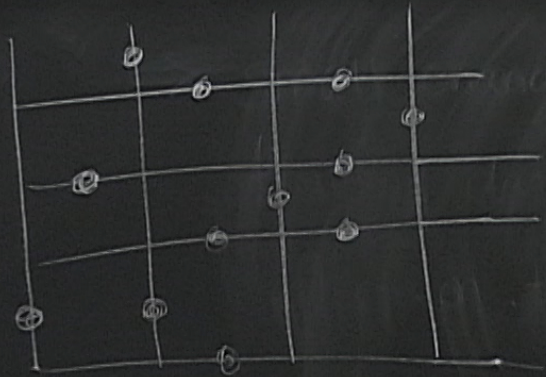


2D torus (square lattice with PBC):



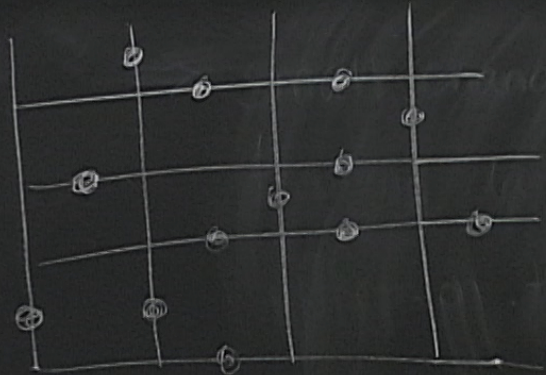
$$L \times L$$
$$L=4$$

2D torus (square lattice with PBC):

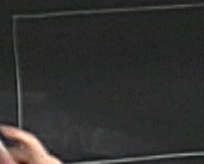


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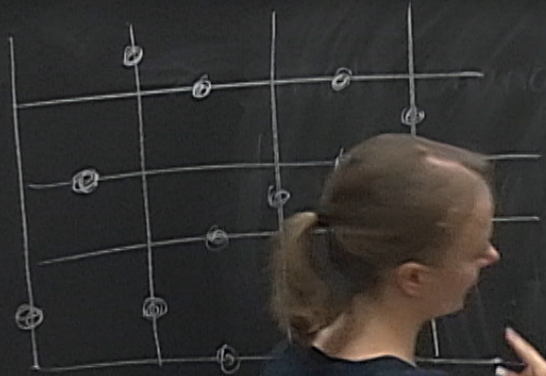
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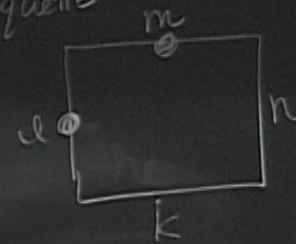


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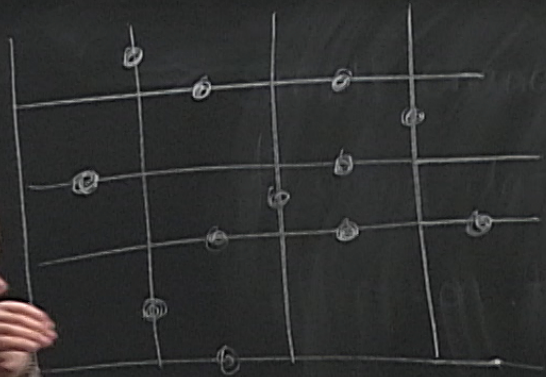


$$L \times L$$
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plaquette

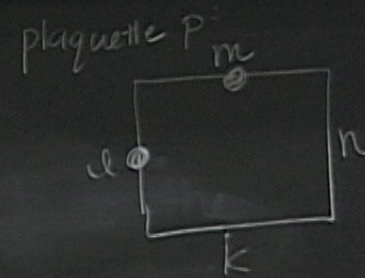


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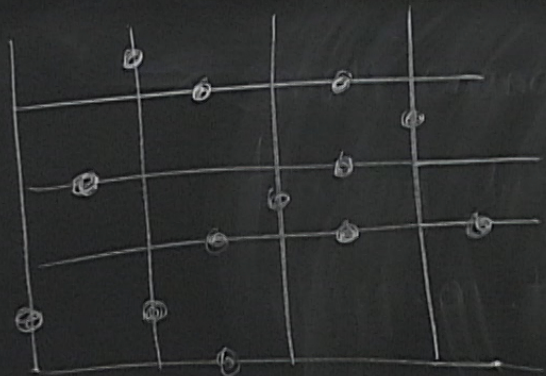
$$L \times L$$

$$L=4$$



$$\prod_{\text{lep}} \delta_p =$$

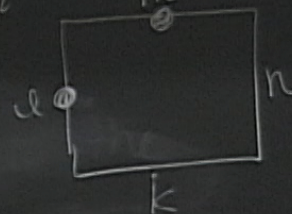
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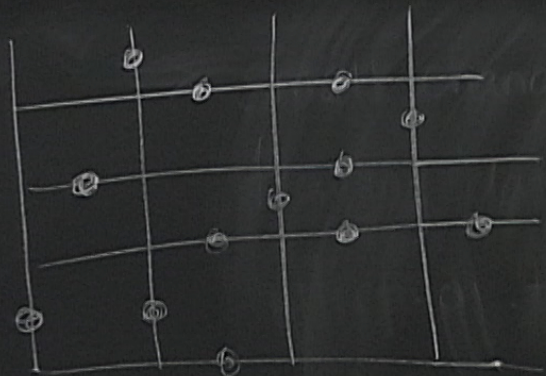
$$L=4$$

plaquette P_m



$$\prod_{i \in P} \sigma_i = \sigma_k \sigma_l \sigma_m \sigma_n$$

2D torus (square lattice with PBC):

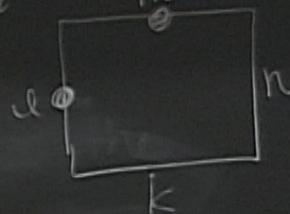


$$L \times L$$

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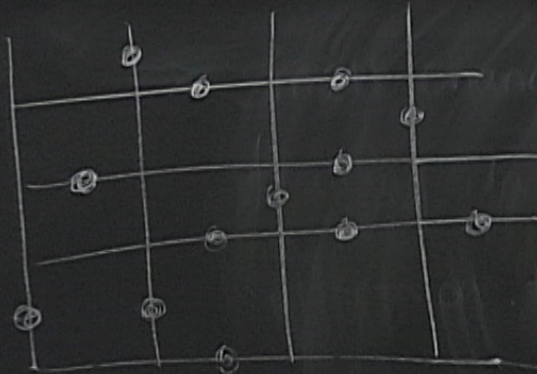


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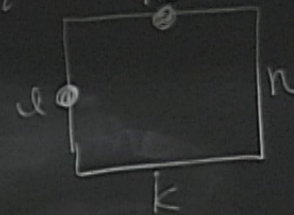
$$L \times L$$

$$L=4$$

$$\# \text{ of spins} = 2L^2$$

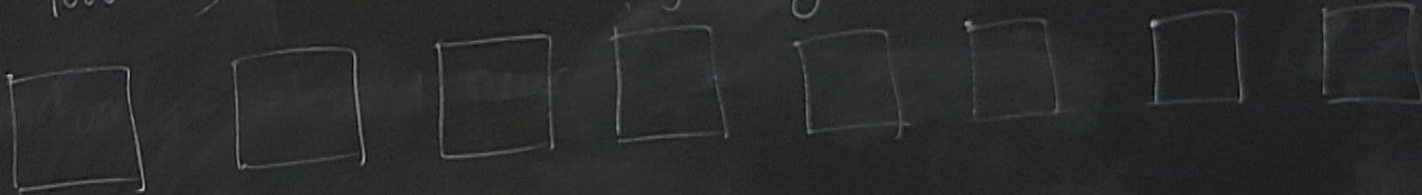


plquette P_m

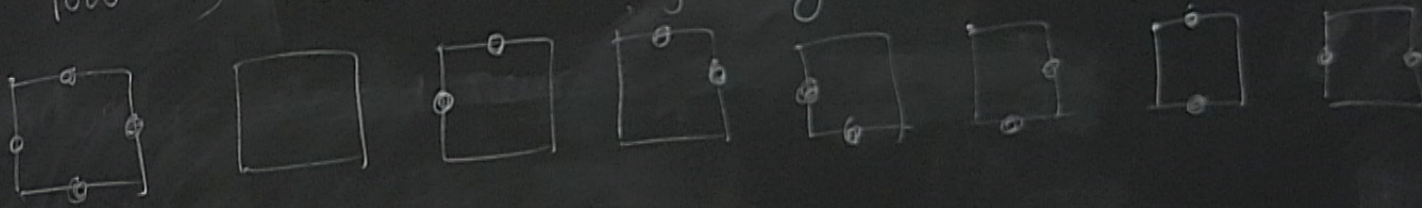


$$\prod_{i \in P} \sigma_i = \sigma_k \sigma_e \sigma_m \sigma_n$$

At low T , there are 8 energetically-favoured plaquettes:

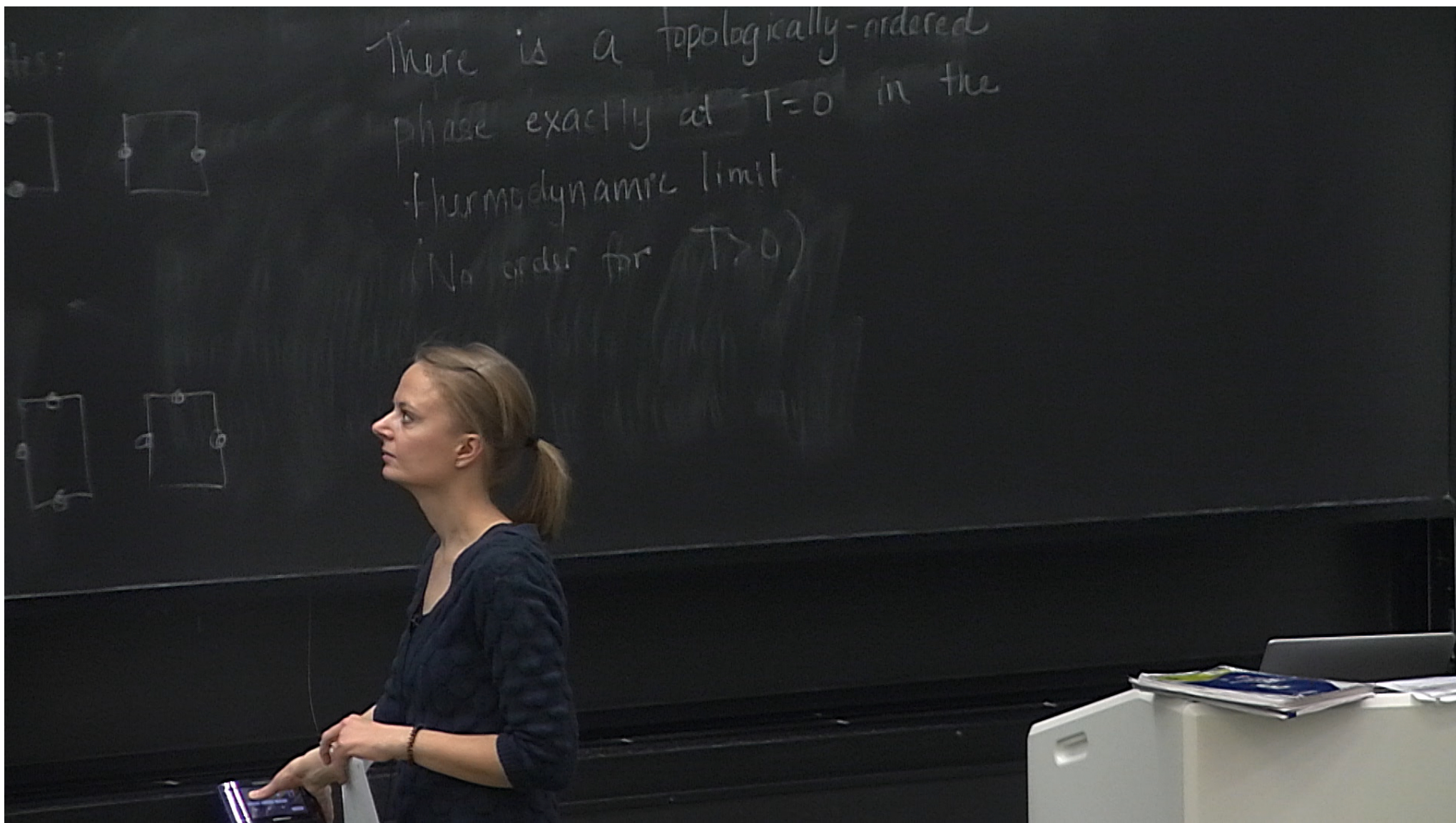


At low T , there are 8 energetically-favoured plaquettes:



And 8 "excited" plaquettes

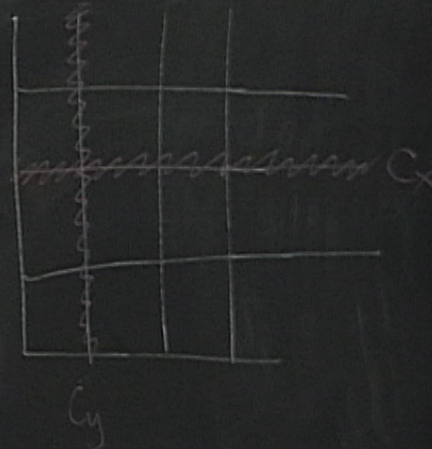




Use a topological quantity W_c as
a measure of this order

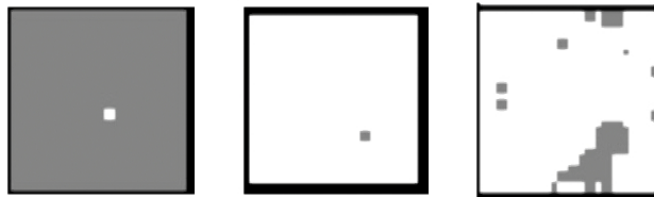
$$W_c = \prod_{i \in C} \sigma_i$$

$$= \pm 1$$



Ising model classification

Ferromagnetic phase:



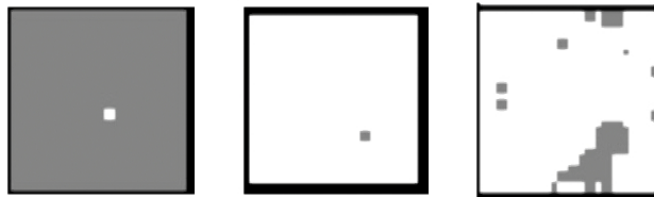
Paramagnetic phase:



Carrasquilla and Melko, arXiv:1605.01735

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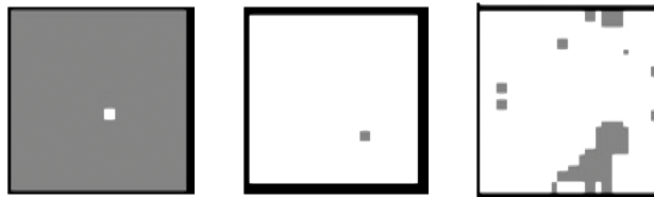
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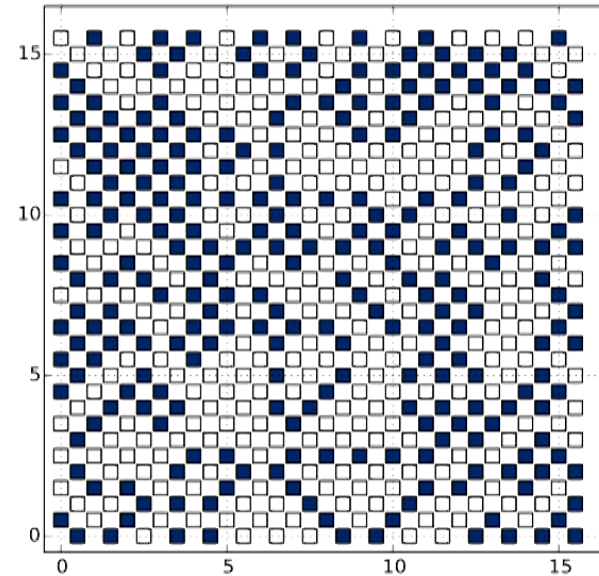
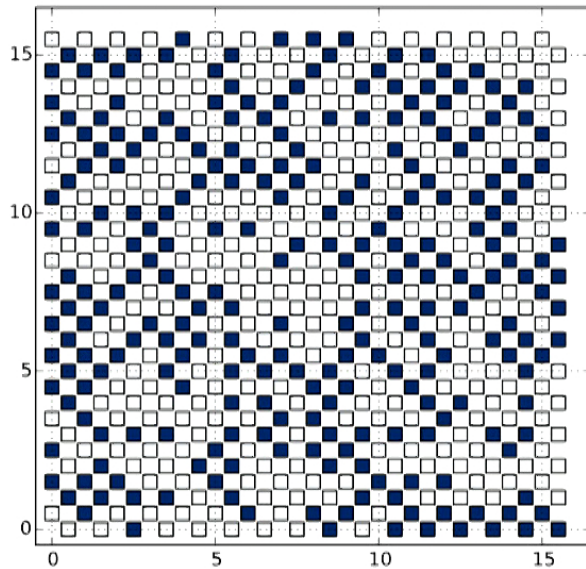


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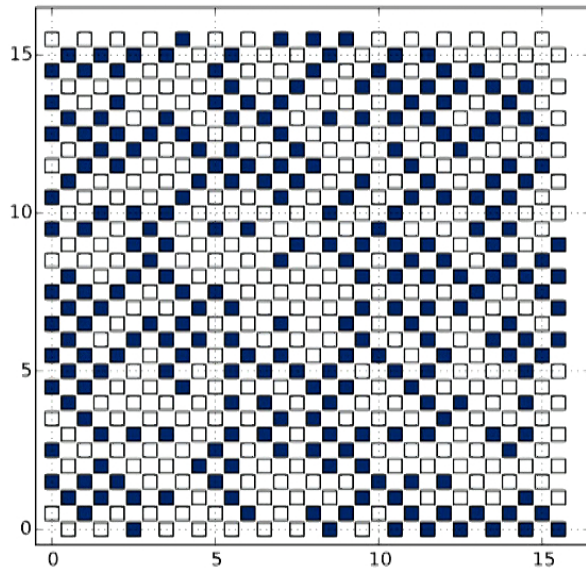
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Ising gauge theory classification

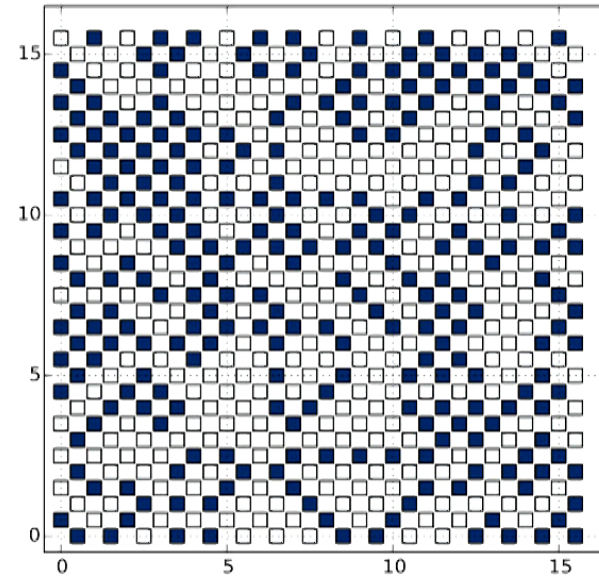


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Ising gauge theory classification



High-temperature state



Ground state

Carrasquilla and Melko, arXiv:1605.01735