Title: 14/15 PSI - Statistical Mechanics - Lecture 1

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Abstract:

Matter organizes itself in distinct phases.

1. Solid - liquid - gas.
2. Ferromagnet - paramagnet.
3. Metal - insulator.

sition

...istinct phases. Phases of matter are distinguished by macroscopic properties

1. Solid has rigidity, while liquid does not.
2. liquid has an interface, while gas does not.
3. FM has spontaneous magnetization, PM does not

...l.

<u>Fundamental idea</u>: The presence of such macroscopic properties is a consequence of <u>ordering</u>.

1. Rigidity of solid is a consequence of ordering of atoms in a periodic crystal structure.

2.

roscopic properties is

2. Ferromagnetism is a consequence
of ordering of atomic magnetic magnetic moments

cture.

Ising model:

In $d>1$ Ising m

Cubic lattice in d-dimensions

$\sigma_i = \pm 1$ - spins.

$$H = -\frac{1}{2}\sum_{ij} J_{ij}\sigma_i\sigma_j$$

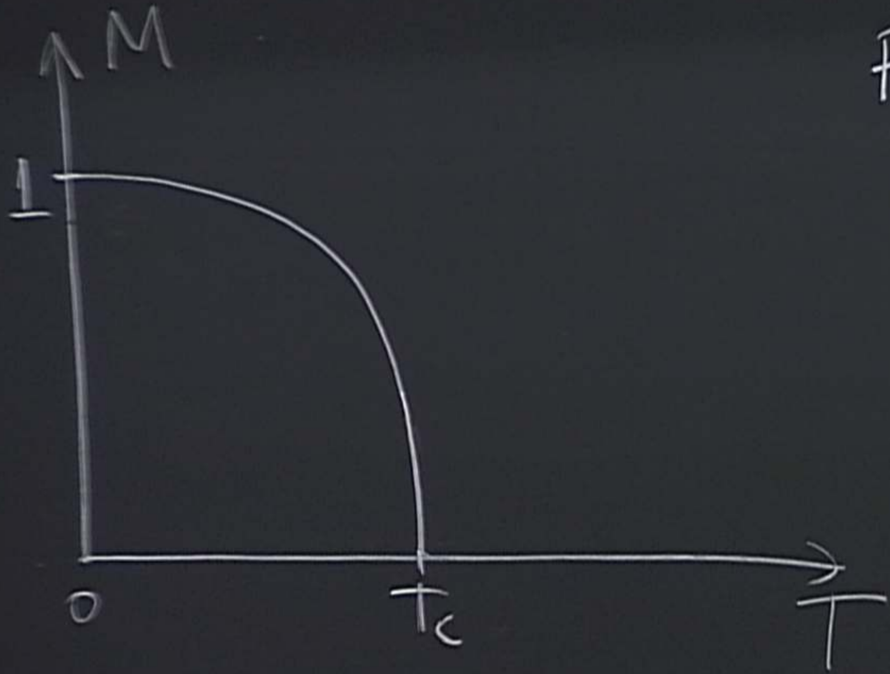
In $d>1$ Ising model exists in 2 phases: FM and PM.

Distinguished by order parameter: $M \neq 0$ in FM phase

$M = 0$ in PM phase

$M = \langle \sigma_i \rangle$ - assuming translational symmetry.

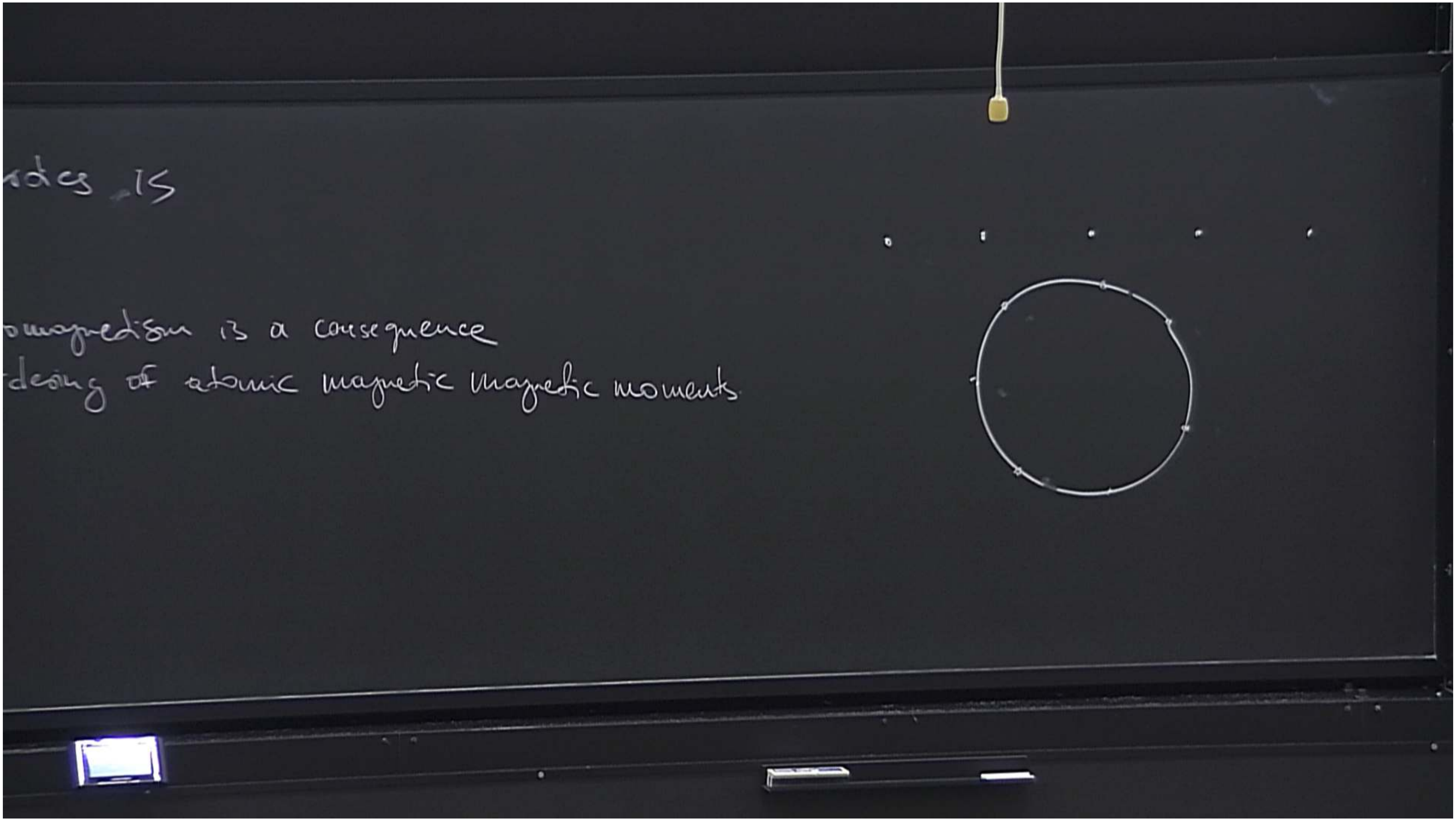
$$\langle \sigma_i \rangle = \frac{1}{Z} \sum_{\{\sigma\}} \sigma_i e^{-\frac{H}{T}}$$



For all i:

$\sigma_i \longrightarrow -\sigma_i$ - symmetry of Ising model.

In FM phase this symmetry is violated spontaneously: - spontaneously broken symmetry.


omagnetism is a consequence
dering of atomic magnetic magnetic moments

$$H = -\frac{1}{2}\sum_{ij} J_{ij}\sigma_i\sigma_j - B\sum_i \sigma_i$$

$B>0$ - prefers $\sigma_i = 1 \Rightarrow$ violates the $\sigma_i \to -\sigma_i$ symmetry.

N - # of lattice sites.

$$H = -\frac{1}{2}\sum_{ij} J_{ij}\sigma_i\sigma_j - BNM$$

$$\frac{P_{M<0}}{P_{M>0}} = \frac{e^{-\frac{NB|M|}{T}}}{e^{\frac{NB|M|}{T}}} = e^{-\frac{2NB|M|}{T}}, \quad \lim_{B\to 0}\lim_{N\to\infty} \frac{P_{M<0}}{P_{M>0}} = 0$$

$$M \neq 0$$

Keep N fixed, while sending $B \to 0$

$$\lim_{N\to\infty}\lim_{B\to 0} \frac{P_{M<0}}{P_{M>0}} = 1 \Rightarrow M=0$$

Phases and phase transitions are well-defined only in the limit $N \to \infty$ - thermodynamic limit.

$$H = -\frac{1}{2}\sum_{ij} J_{ij}\sigma_i\sigma_j - B\sum_i \sigma_i$$

$B>0$ - prefers $\sigma_i = 1 \Rightarrow$ violates the $\sigma_i \to -\sigma_i$ symmetry.

N - # of lattice sites.

$$H = -\frac{1}{2}\sum_{ij} J_{ij}\sigma_i\sigma_j - BNM$$

$$Z = \sum_{\{\sigma\}} e^{-\frac{H}{T}}$$

$$\frac{P_{M<0}}{P_{M>0}} =$$

Keep N f

$$\lim_{N\to\infty}\lim_{B\to 0} \frac{P_{M}}{P_{M}}$$

– mean field theory (MFT)

M

$$= (\sigma_i - M)\cdot\cancel{(\sigma_j - M)}^{\to 0} + M(\sigma_i - M + \sigma_j - M) + M^2 \simeq$$

$$\simeq M(\sigma_i + \sigma_j) - 2M^2 + M^2 = M(\sigma_i + \sigma_j) - M^2$$

...at

...all

Simplest description of phase transition – mean field theory (

$$\sigma_i = \sigma_i - \langle\sigma_i\rangle + \langle\sigma_i\rangle = \sigma_i - M + M$$

assume that this is small

$$\sigma_i \sigma_j = (\sigma_i - M + M)\cdot(\sigma_j - M + M) =$$

$$= \cancel{(\sigma_i - M)\cdot(\sigma_j - M}$$

$$\simeq M(\sigma_i +$$

$$H = -\frac{1}{2}\sum_{ij} J_{ij} M(\sigma_i + \sigma_j) + \frac{1}{2}\sum_{ij} J_{ij} M^2$$

$$J = \sum_{j} J_{ij}$$ - assume J is finite

$$H = -JM\sum_{i}\sigma_i + \frac{1}{2}NJM^2$$

$$Z = \sum_{\{\sigma\}} e^{-\frac{H}{T}} = \sum_{\{\sigma\}} e^{\frac{JM}{T}\sum_i \sigma_i}\, e^{-\frac{NJM^2}{2T}}$$

$$= e^{-\frac{NJM^2}{2T}} \prod_{i=1}^{N} \sum_{\sigma_i=\pm 1} e^{\frac{JM}{T}\sigma_i} = e^{-\frac{NJM^2}{2T}} \left[e^{\frac{JM}{T}} + e^{-\frac{JM}{T}} \right]^N =$$

$$= e^{-\frac{NJM^2}{2T}} \left[2\cosh\left(\frac{JM}{T}\right) \right]^N$$

Helmholtz free energy:

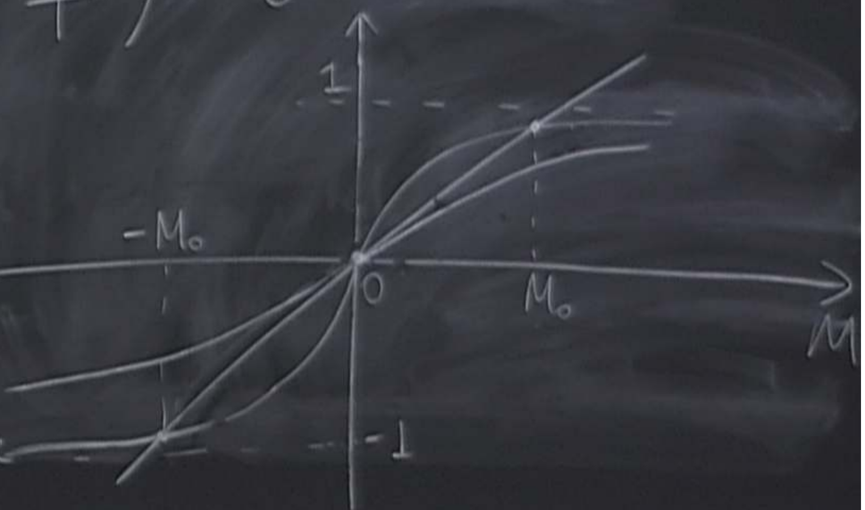
$$F = -T \ln Z = \frac{NJM^2}{2} - TN \ln\left[2\cosh\left(\frac{JM}{T}\right)\right]$$

$$\frac{\partial F}{\partial M} = \cancel{N}JM - \cancel{N}J\tanh\left(\frac{JM}{T}\right) = 0$$

$$M = \tanh\left(\frac{JM}{T}\right)$$

$$\tanh\left(\frac{JM}{T}\right) \simeq \frac{JM}{T}$$

$\frac{J}{T} > 1$ - have nontrivial solutions - FM phase



Helmholtz free energy:

$$F = -T \ln Z = \frac{NJM^2}{2} - TN \ln\left[2\cosh\left(\frac{JM}{T}\right)\right] ;$$

Minimize F as a function of M.

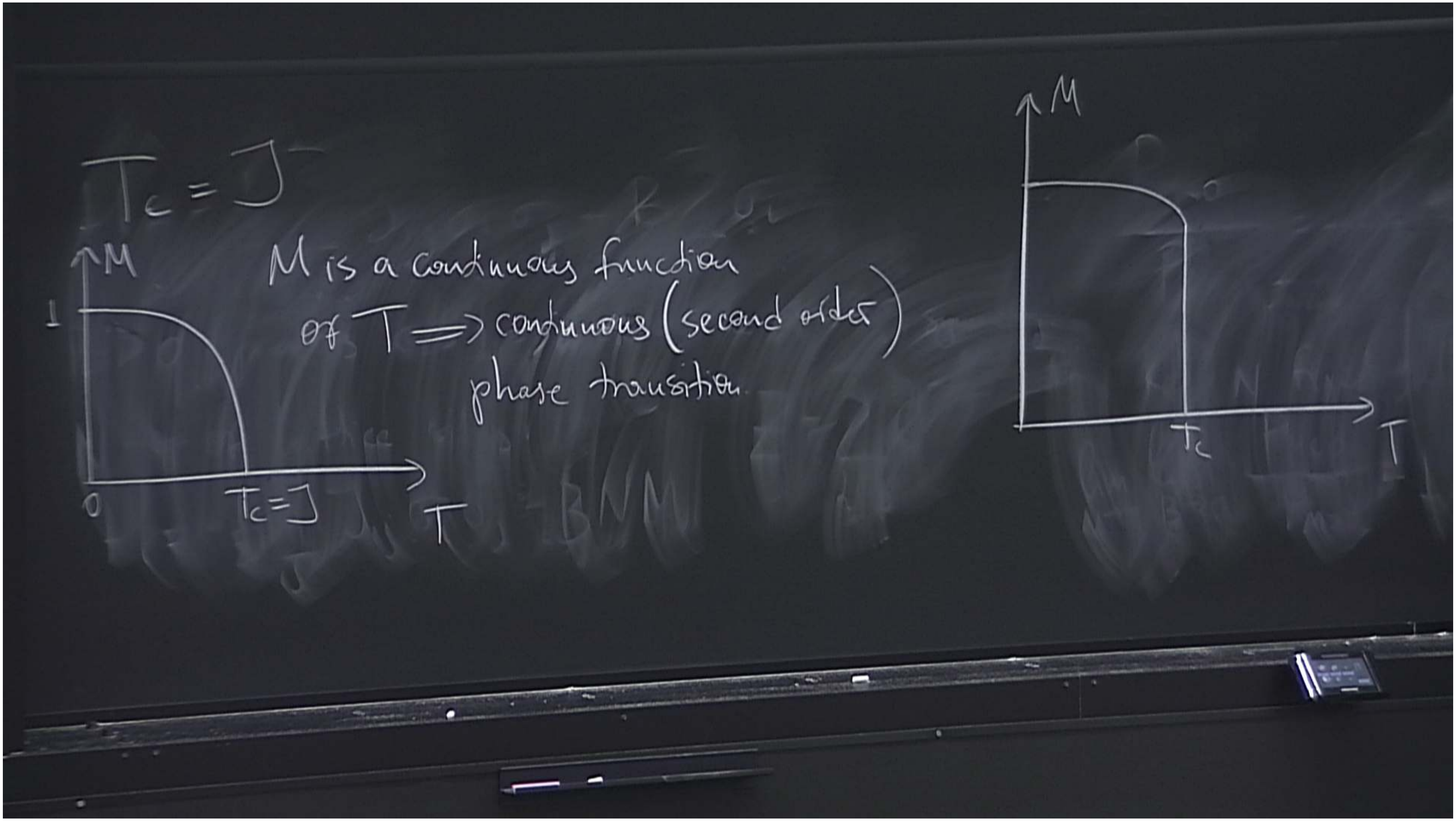
$\frac{J}{T} < 1$ – only $M=0$ is the solution – PM phase

$$\frac{\partial F}{\partial M} = N$$

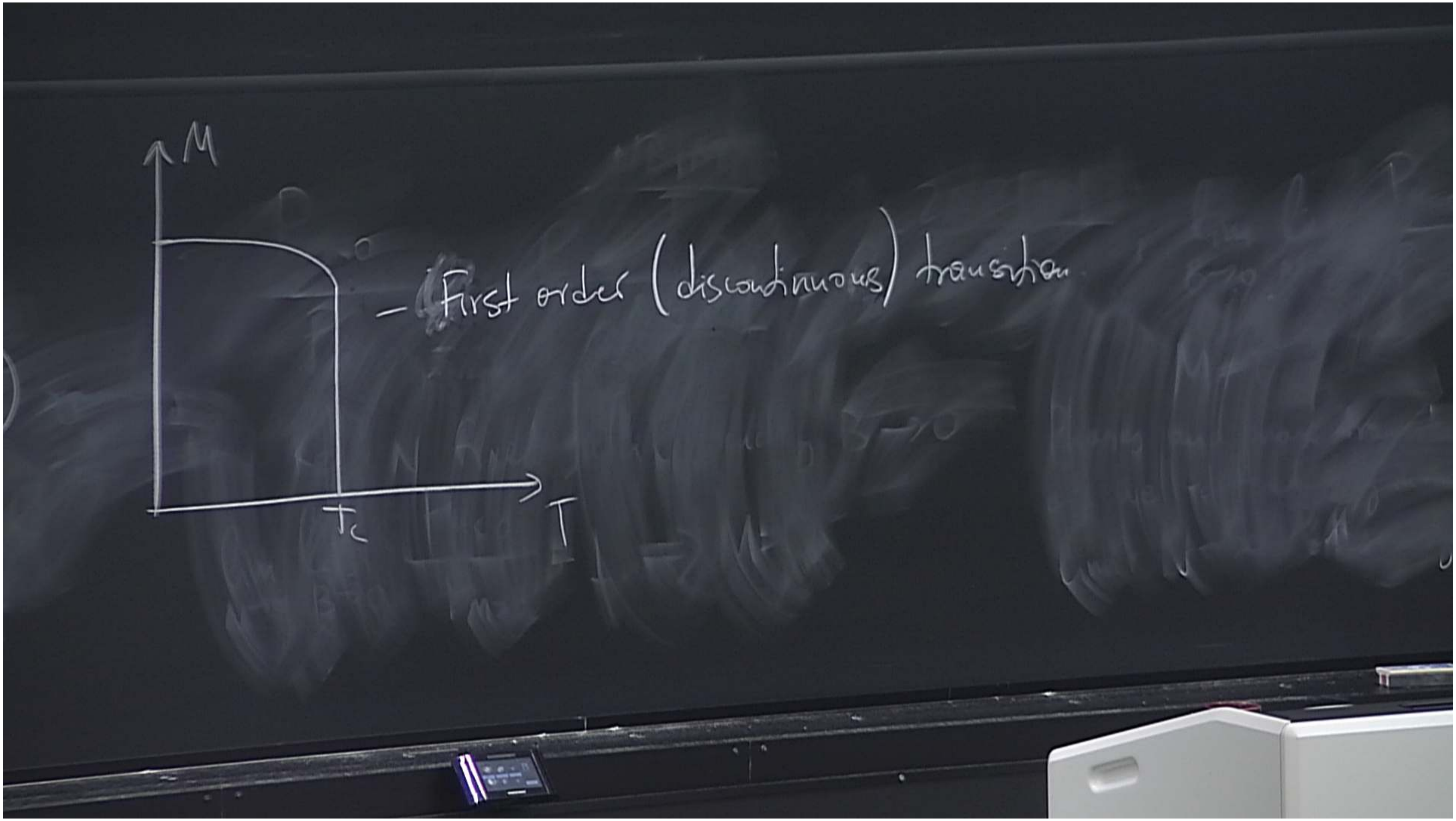
M

$\tanh\left(\frac{JM}{T}\right) \approx \left(\frac{J}{\ }\right.$

$\frac{J}{T} > 1$ – have nontr



Tc = J
M
1
0
Tc=J
T
M is a continuous function
of T ⟹ continuous (second order)
phase transition
M
Tc
T


M
T
Tc
— First order (discontinuous) transition