Title: 2016/2017 Statistical Mechanics 2 - Roger Melko - Lecture 2

Date: Jan 06, 2017 10:30 AM

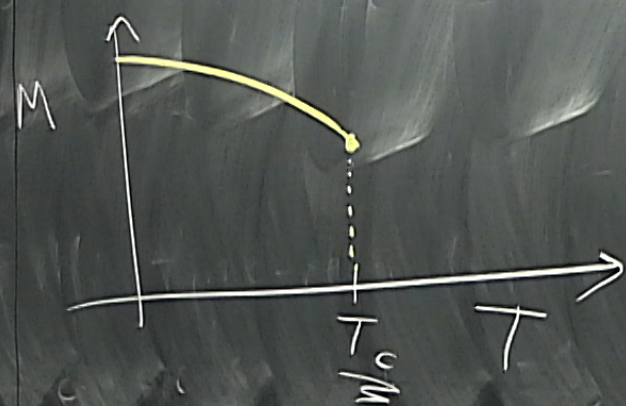
URL: http://pirsa.org/17010048

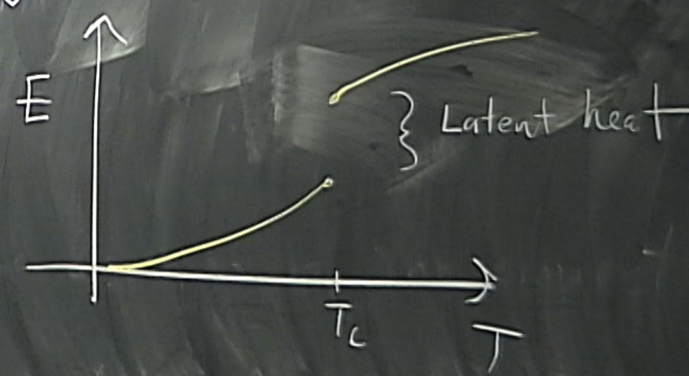
Abstract:

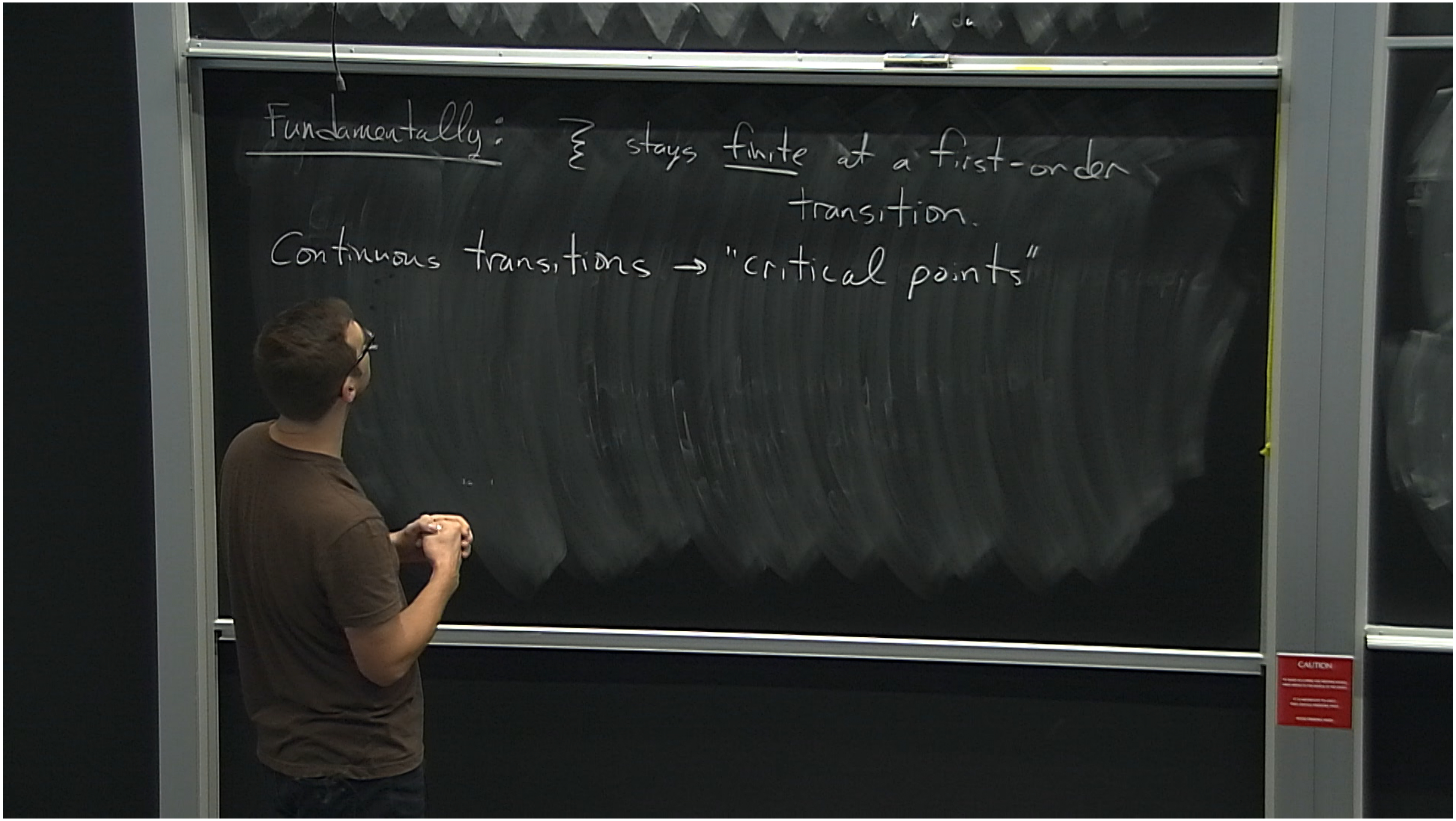
Phase transitions

classify as "First order" or "continuous"

First order: discontinuity in e.g.





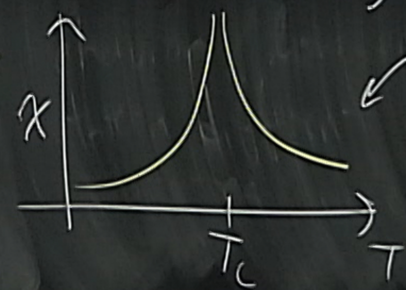

Fundamentally: ξ stays finite at a first-order transition.
Continuous transitions → "critical points"

transition.

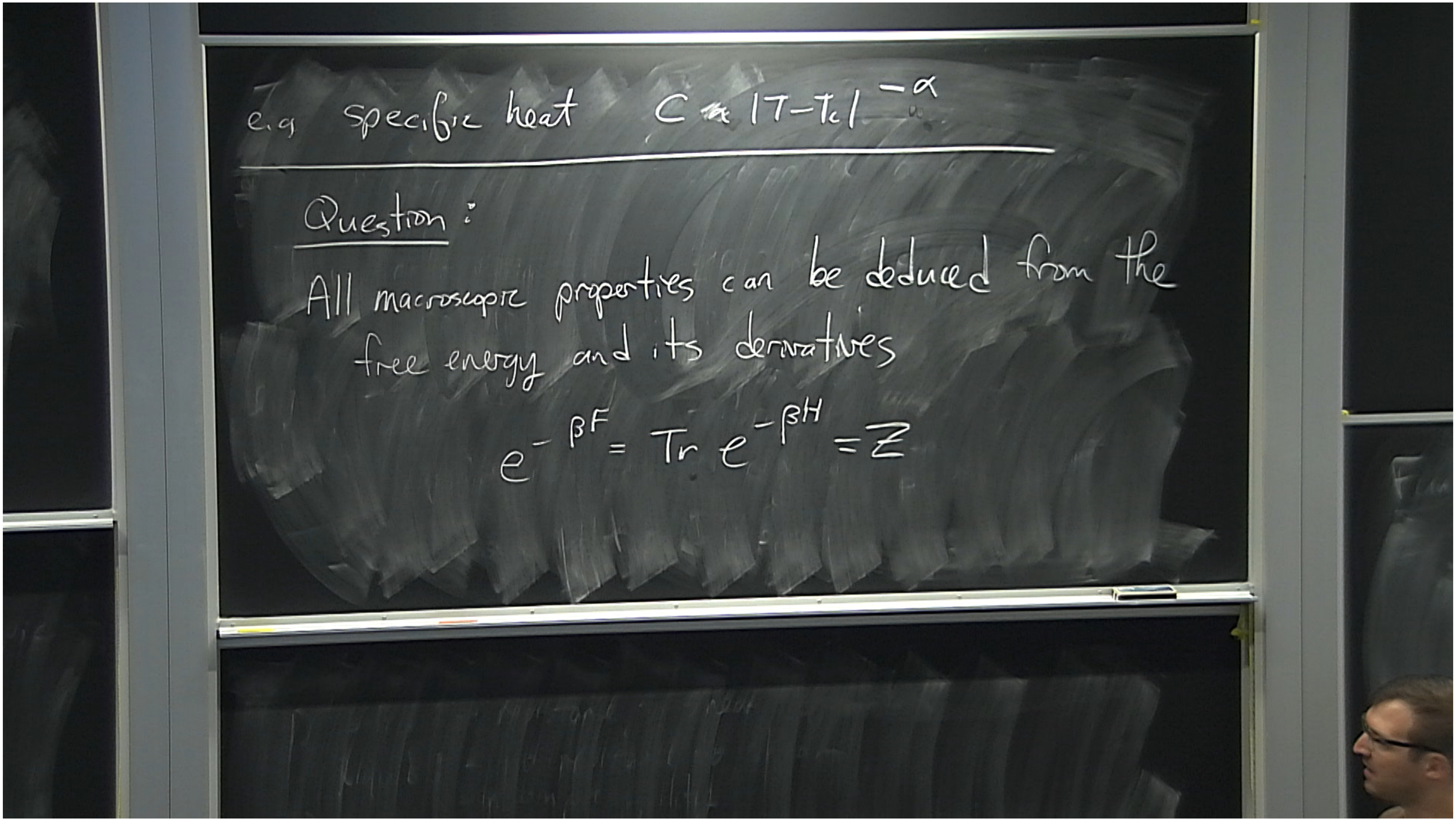
Continuous transitions → "critical points"

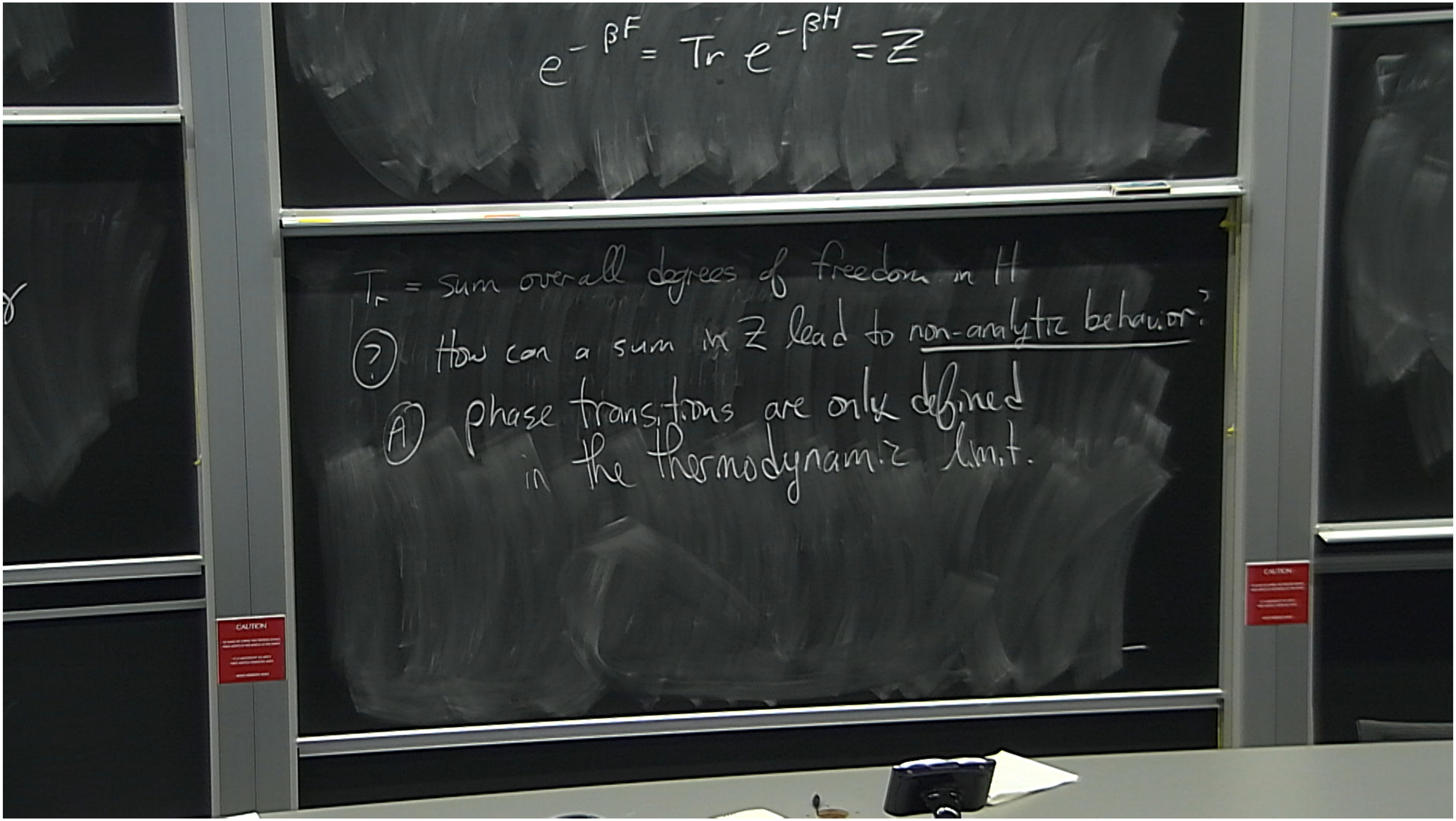
(fundamental : $\xi \to \infty$)

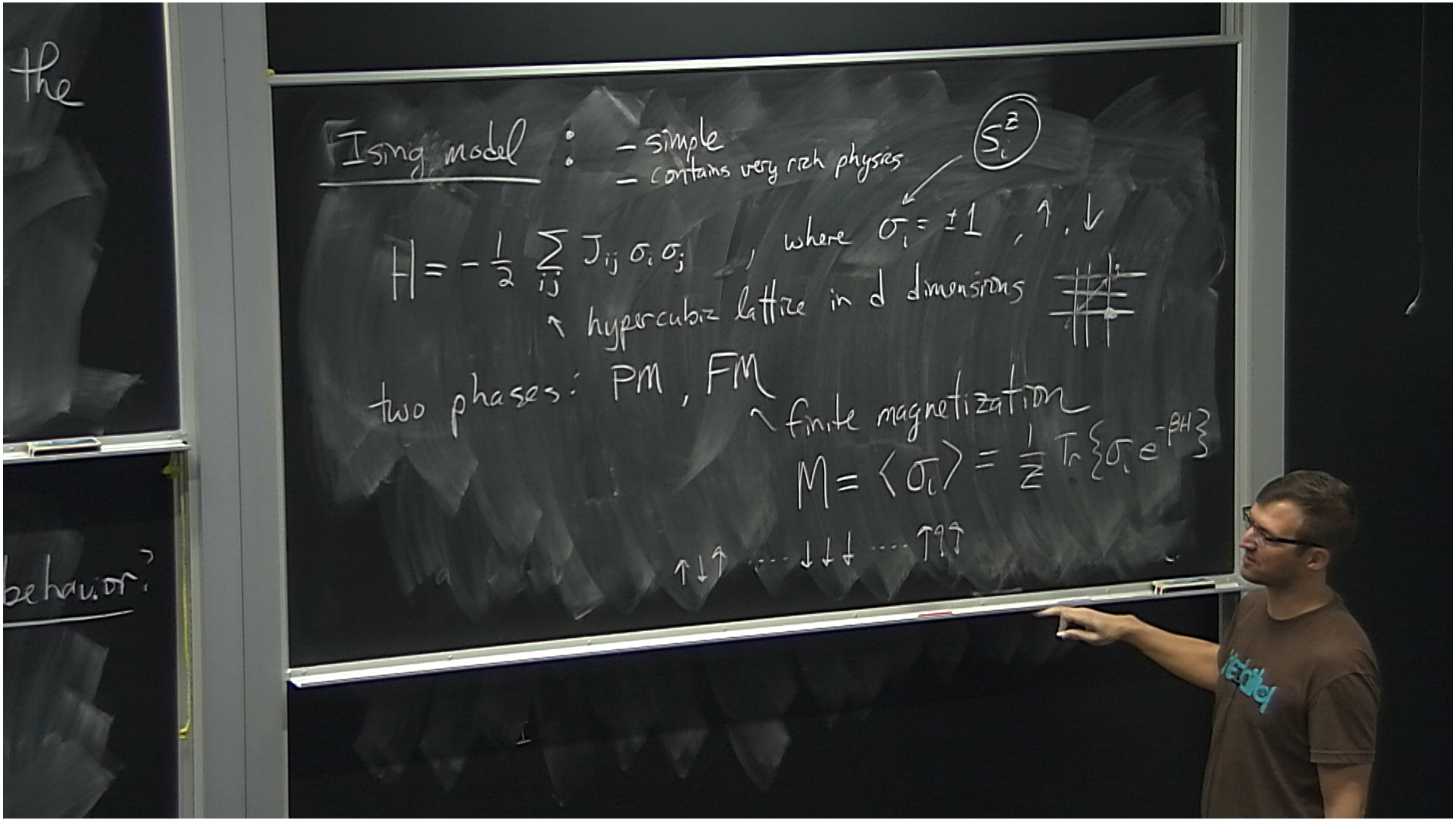
e.g. susceptibility



$\chi \propto |T_c - T|^{-\gamma}$


e.g. specific heat $C \propto |T-T_c|^{-\alpha}$
Question:
All macroscopic properties can be deduced from the free energy and its derivatives
$e^{-\beta F} = \mathrm{Tr}\, e^{-\beta H} = Z$

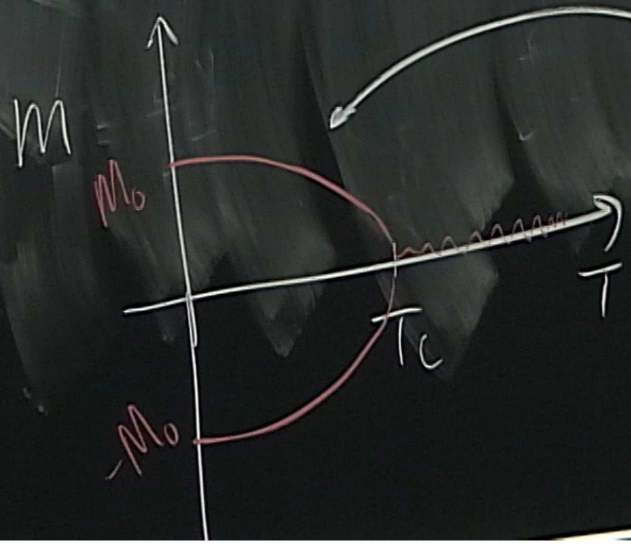

$e^{-\beta F} = \mathrm{Tr}\, e^{-\beta H} = Z$
Tr = sum overall degrees of freedom in H
? How can a sum in Z lead to non-analytic behavior?
A phase transitions are only defined in the thermodynamic limit.


the
Ising model : - simple
- contains very rich physics
S_i^z
$H = -\frac{1}{2} \sum_{ij} J_{ij} \sigma_i \sigma_j$, where $\sigma_i = \pm 1$, ↑, ↓
hypercubic lattice in d dimensions
two phases: PM , FM
finite magnetization
$M = \langle \sigma_i \rangle = \frac{1}{Z} \mathrm{Tr}\{\sigma_i e^{-\beta H}\}$
↑↓↑ .... ↓↓↓ .... ↑↑↑
behavior?

<u>Note</u>: the Ising Hamiltonian is invariant under time-reversal

$\sigma_i \longrightarrow -\sigma_i \qquad H \to H$

The groundstate is a FM: $\uparrow\uparrow\uparrow\uparrow\uparrow$ <u>or</u> $\downarrow\downarrow\downarrow\downarrow\downarrow$



<u>spontaneous</u> symmetry breaking

Although the Hamiltonian is invariant under time reversal symmetry, the FM state is <u>not</u>.

<u>Add a magnetic field</u>

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

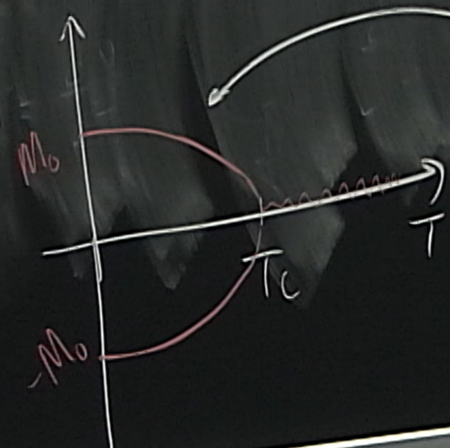
Consider a finite-size system with N spins:

For large N, $M \simeq \frac{1}{N}\sum_i \sigma_i$

Note: the Ising Hamiltonian is invariant under time-reversal

$\sigma_i \longrightarrow -\sigma_i \qquad H \rightarrow H \qquad \vec{B}$

The groundstate is a FM: ↑↑↑↑↑ or ↓↓↓↓↓



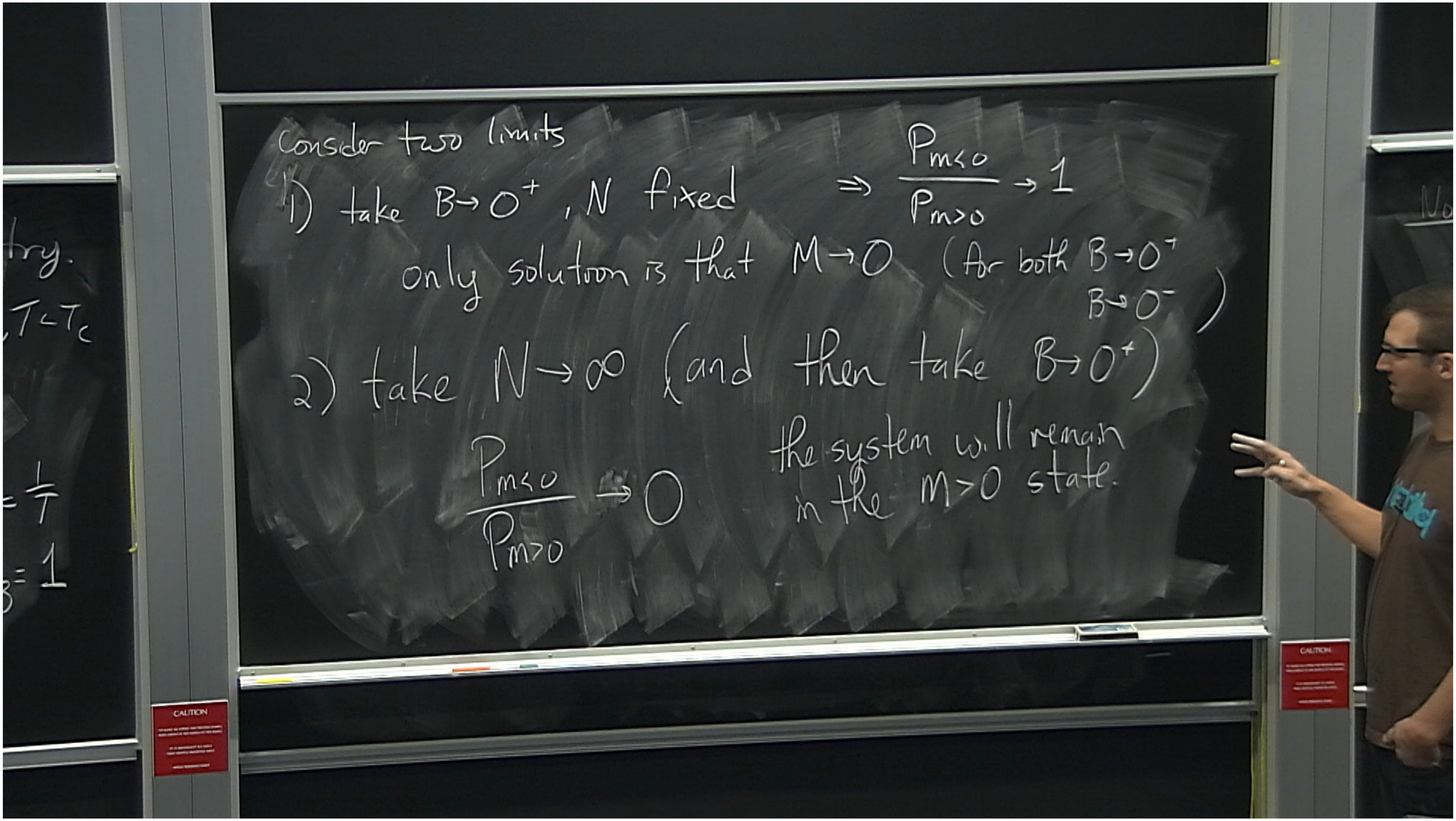
spontaneous symmetry breaking

The B term explicitly breaks time-reversal symmetry.

- if $B>0$ the system will prefer $M>0$, $T<T_c$
- " $B<0$ " " " " $M<0$

Consider the "relative probability"

$$\frac{P_{M<0}}{P_{M>0}} = \frac{e^{-\beta(+BNM)}}{e^{-\beta(-BNM)}} = e^{-\frac{2BNM}{T}} \ll 1 \text{ low } T \qquad \beta = \frac{1}{T}, \quad k_B = 1$$

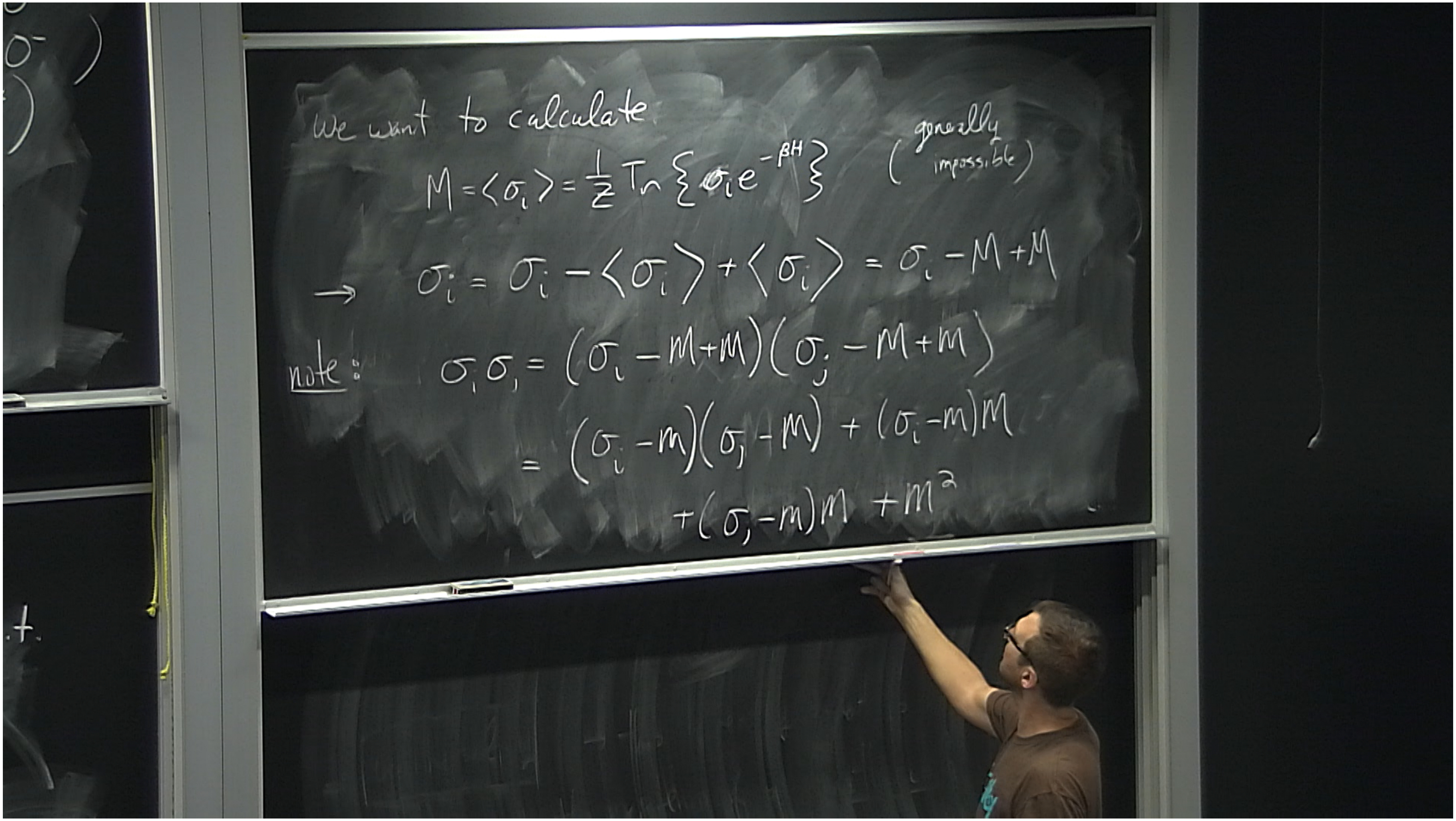

Consider two limits
1) take $B \to 0^+$, N fixed $\Rightarrow \frac{P_{m<0}}{P_{m>0}} \to 1$
only solution is that $M \to 0$ (for both $B \to 0^+$, $B \to 0^-$)
2) take $N \to \infty$ (and then take $B \to 0^+$)
$\frac{P_{m<0}}{P_{m>0}} \to 0$
the system will remain in the $M>0$ state.

Moral: spontaneous symmetry breaking is only possible in the thermodynamic limit.

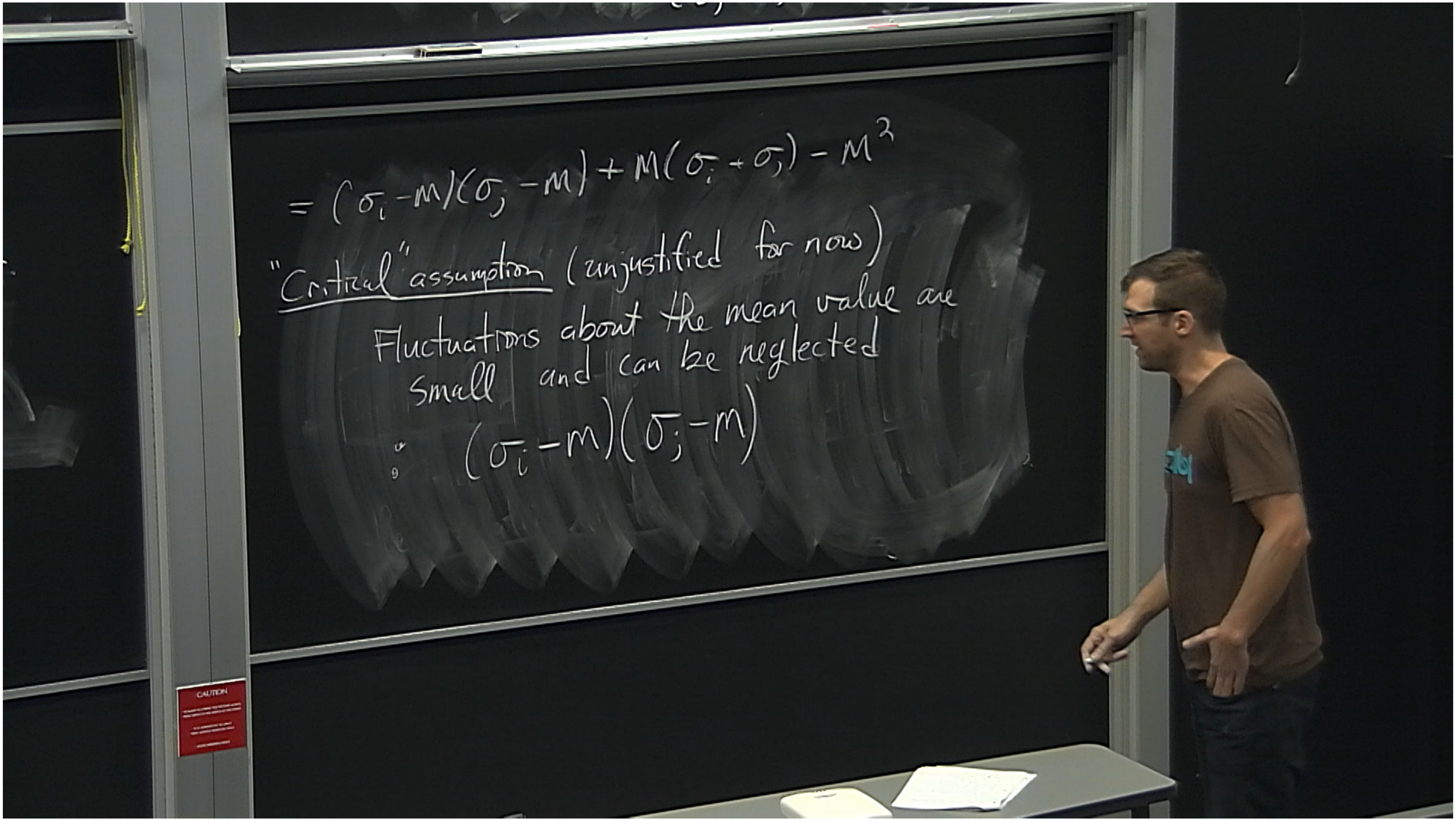
Mean-field theory of the Ising model.

→ 1D homework } exact solutions
→ 2D Onsager }

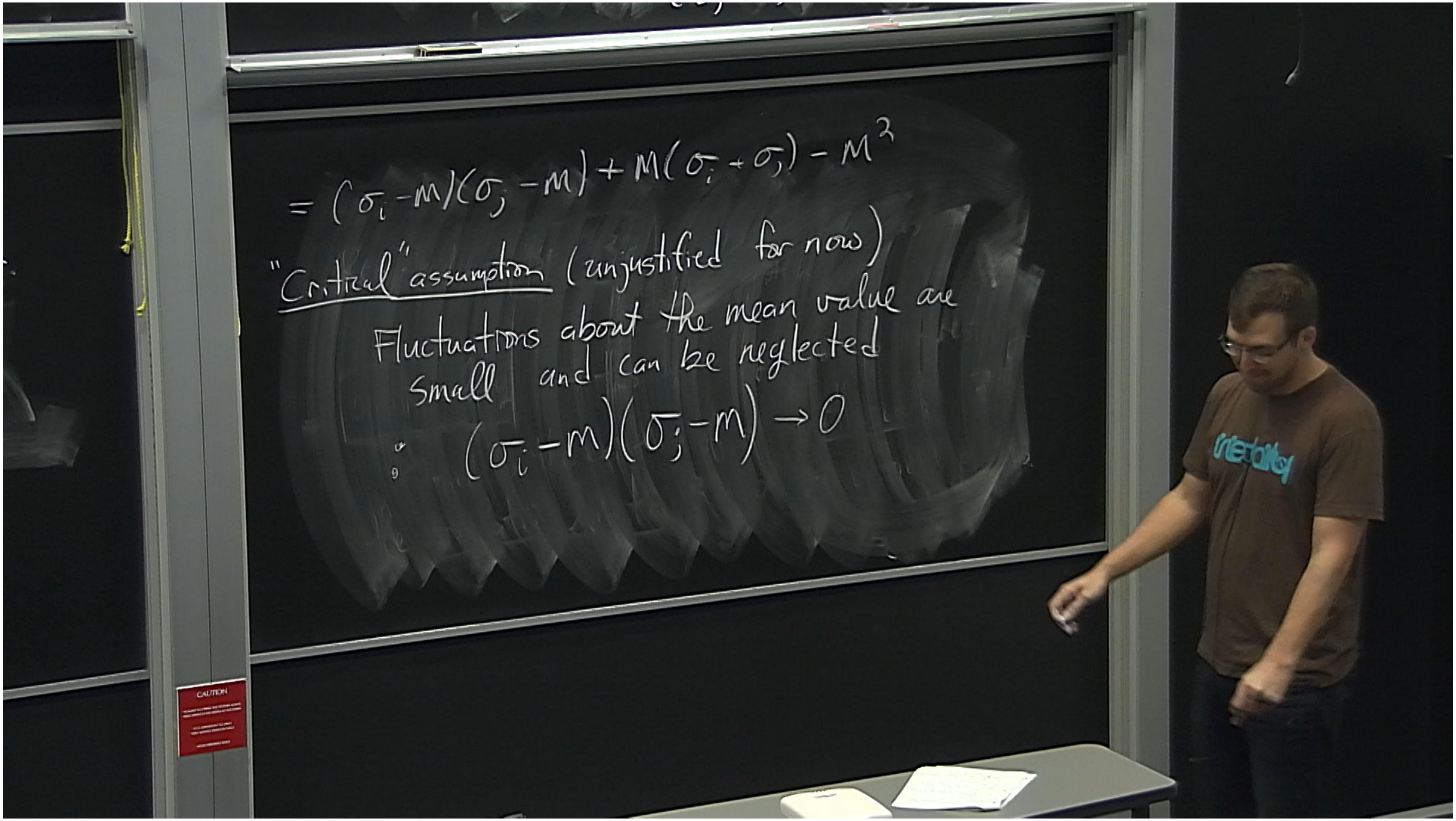
MFT is an approximation.



We want to calculate
$M = \langle \sigma_i \rangle = \frac{1}{Z} \mathrm{Tr} \{ \sigma_i e^{-\beta H} \}$
(generally impossible)
$\rightarrow \sigma_i = \sigma_i - \langle \sigma_i \rangle + \langle \sigma_i \rangle = \sigma_i - M + M$
note:
$\sigma_i \sigma_j = (\sigma_i - M + M)(\sigma_j - M + M)$
$= (\sigma_i - M)(\sigma_j - M) + (\sigma_i - M)M$
$+ (\sigma_j - M)M + M^2$



$= (\sigma_i - m)(\sigma_j - m) + m(\sigma_i + \sigma_j) - m^2$
"Critical" assumption (unjustified for now)
Fluctuations about the mean value are small and can be neglected
$(\sigma_i - m)(\sigma_j - m)$


$= (\sigma_i - m)(\sigma_j - m) + m(\sigma_i + \sigma_j) - m^2$
"Critical" assumption (unjustified for now)
Fluctuations about the mean value are small and can be neglected
$(\sigma_i - m)(\sigma_j - m) \to 0$
CAUTION

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

Let $\sum_j J_{ij} \equiv J_i \equiv J$ assuming translational invariance.

then $$H = -MJ\sum_i \sigma_i + \frac{1}{2} N J M^2$$

This allows us to calculate the free energy

$$F = -T \ln Z$$

The B term ex

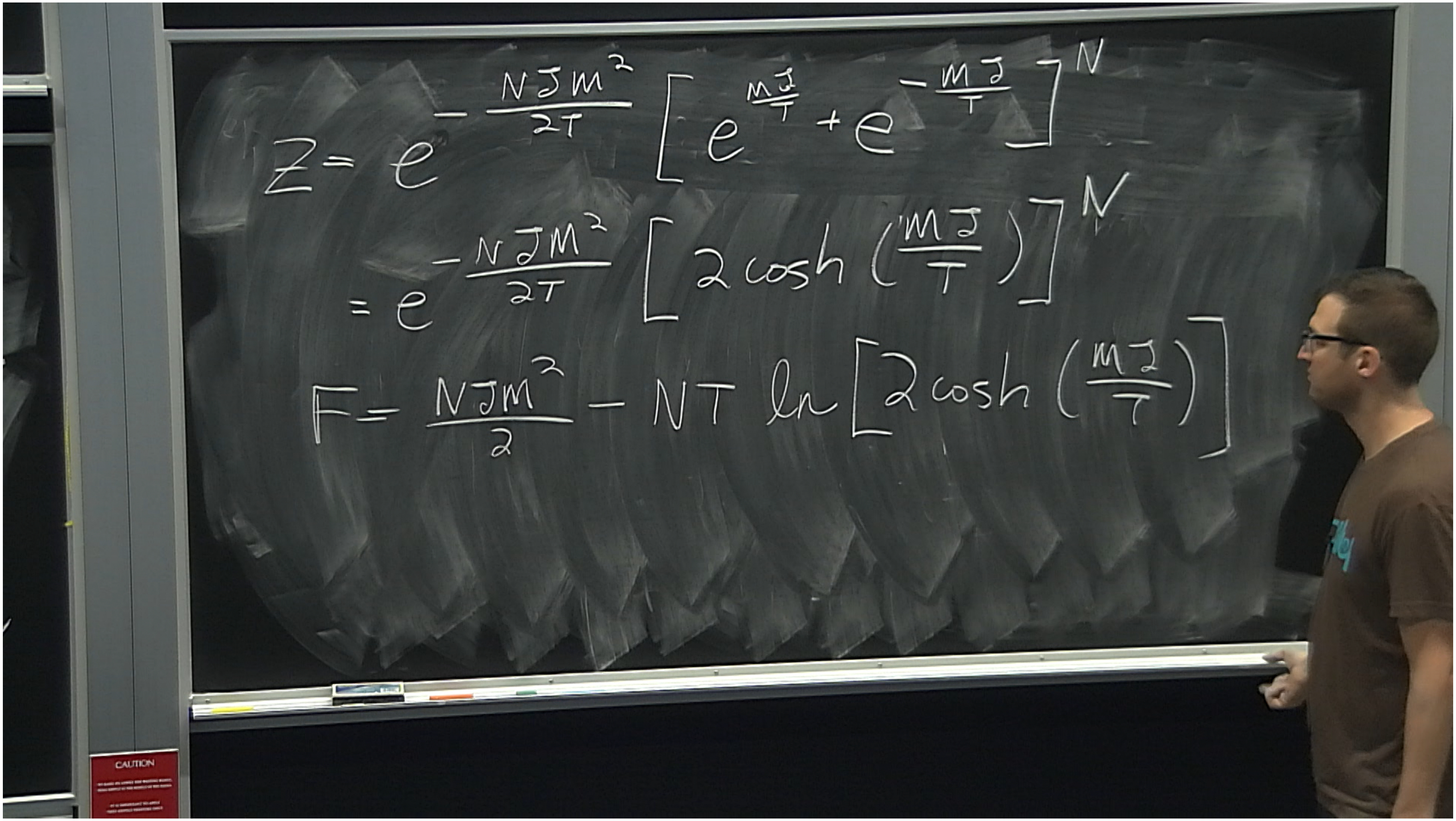
$$Z = \mathrm{Tr}\left\{ e^{-\beta H} \right\}$$

$$= \underbrace{\sum_{\sigma_1 = \pm 1} \sum_{\sigma_2 = \pm 1} \sum_{\sigma_3 = \pm 1} \cdots \sum_{\sigma_N = \pm 1}}_{\sum_{\{\sigma_i = \pm 1\}} \text{ or } \prod_{i=1}^{N} \sum_{\sigma_i = \pm 1}} e^{-\beta H}$$

$$Z = \mathrm{Tr}\left\{ e^{-\beta H} \right\}$$

$$= \underbrace{\sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \sum_{\sigma_3=\pm 1} \cdots \sum_{\sigma_N=\pm 1}}_{\sum_{\{\sigma_i=\pm 1\}} \text{ or } \prod_{i=1}^{N} \sum_{\sigma_i=\pm 1}} e^{-\beta H}$$

$$Z = e^{-\frac{NJM^2}{2T}} \cdot \sum_{\sigma_1=\pm 1} e^{\frac{mJ}{T}\sigma_1} \cdot \sum_{\sigma_2=\pm 1} e^{\frac{mJ}{T}\sigma_2} \cdots \sum_{\sigma_N \pm 1} e^{\frac{mJ}{T}\sigma_N}$$

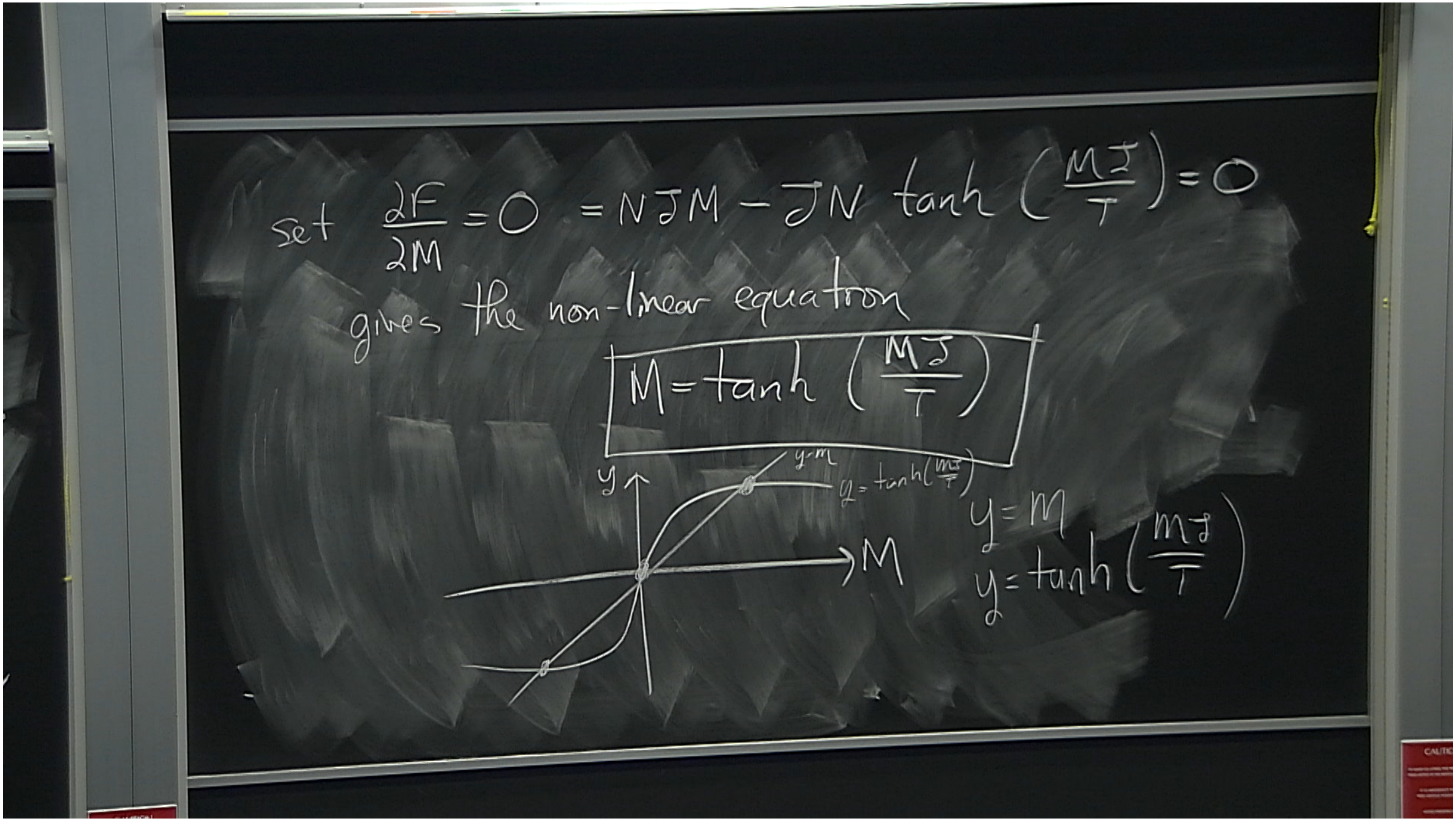

$Z = e^{-\frac{NJm^2}{2T}}\left[e^{\frac{mJ}{T}} + e^{-\frac{mJ}{T}}\right]^N$
$= e^{-\frac{NJm^2}{2T}}\left[2\cosh\left(\frac{mJ}{T}\right)\right]^N$
$F = \frac{NJm^2}{2} - NT\ln\left[2\cosh\left(\frac{mJ}{T}\right)\right]$
CAUTION

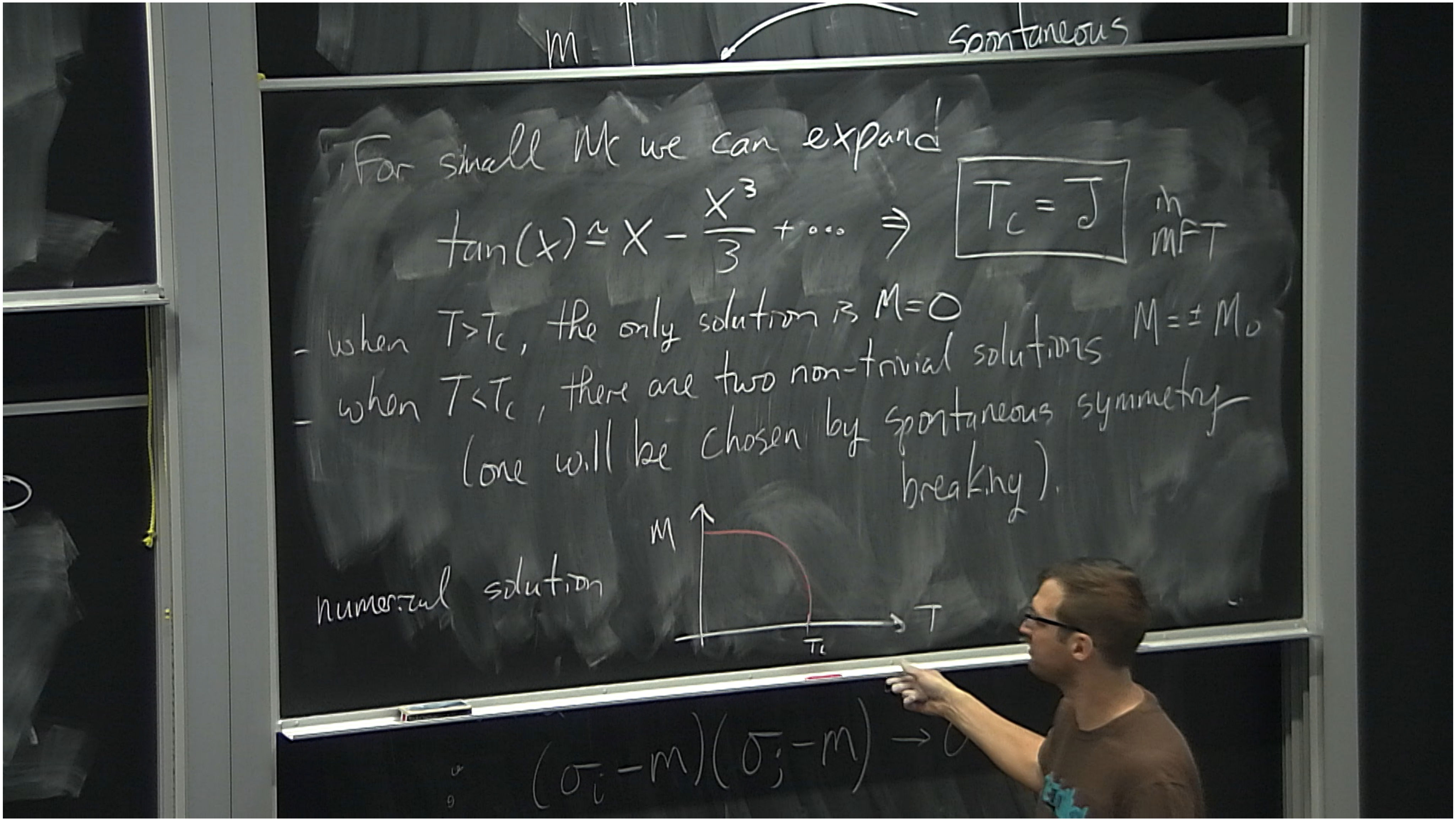
$$Z = e^{\cdots} \left[\cdots \right]$$

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

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

Now M is determined by requiring that it minimizes the free energy


set $\frac{\partial F}{\partial M} = 0 = NJM - JN \tanh\left(\frac{MJ}{T}\right) = 0$
gives the non-linear equation
$\boxed{M = \tanh\left(\frac{MJ}{T}\right)}$
y
y=m
$y = \tanh\left(\frac{mJ}{T}\right)$
M
$y = m$
$y = \tanh\left(\frac{mJ}{T}\right)$

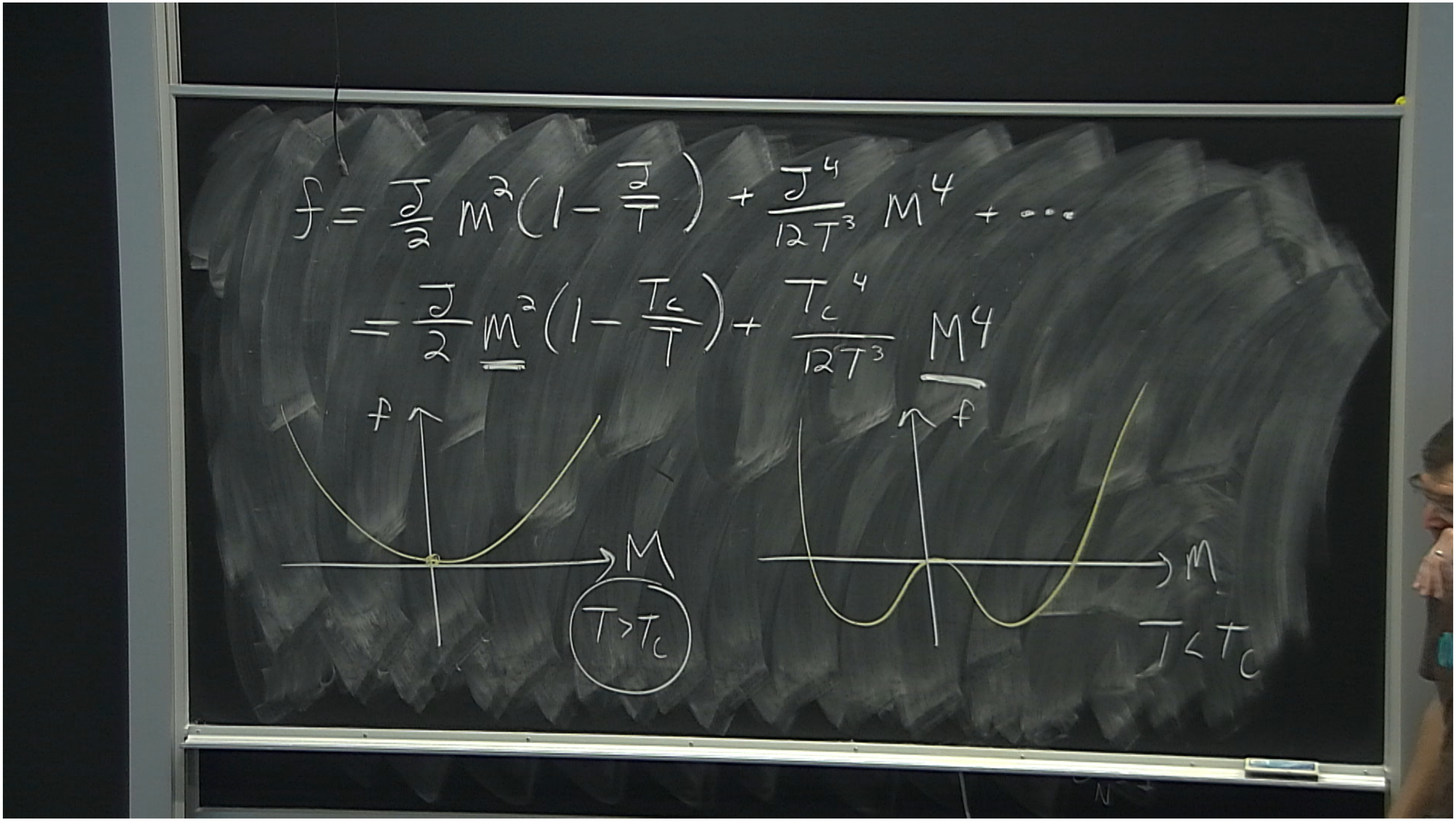

Spontaneous
For small M we can expand
tan(x) ≃ X - X^3/3 + ... ⇒
T_c = J
in MFT
- when T>T_c, the only solution is M=0
- when T<T_c, there are two non-trivial solutions M=±M_0
(one will be chosen by spontaneous symmetry breaking).
numerical solution
M
T
T_c
(σ_i - m)(σ_j - m) →

Near T_c M is small and we can expand the free energy in a Taylor series

$$f = \frac{F}{N} = \frac{1}{2} J M^2 - T \ln\left[2\cosh(\beta M J)\right]$$

$$\ln\left[2\cosh x\right] \simeq \ln 2 + \frac{x^2}{2} - \frac{x^4}{12} + \frac{x^6}{45}$$

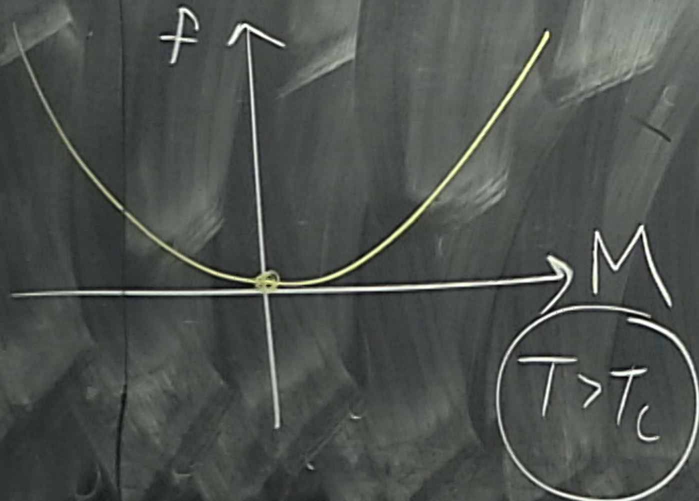
$$f = \frac{1}{2} J M^2 - \frac{1}{2} T (\beta M J)^2 + \frac{1}{12} T (\beta M J)^4 + \cdots + \text{const.}$$

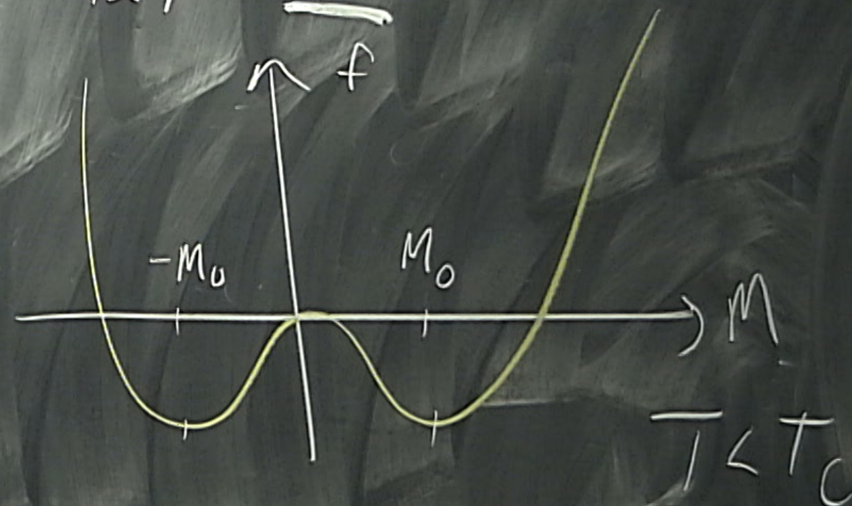


$f = \frac{J}{2} M^2 \left(1 - \frac{J}{T}\right) + \frac{J^4}{12T^3} M^4 + \cdots$
$= \frac{J}{2} M^2 \left(1 - \frac{T_c}{T}\right) + \frac{T_c^4}{12T^3} M^4$
f
M
$T > T_c$
f
M
$T < T_c$

$$f = \frac{J}{2} M^2 \left(1 - \frac{J}{T}\right) + \frac{J^4}{12T^3} M^4 + \cdots$$

$$= \frac{J}{2} \underline{M}^2 \left(1 - \frac{T_c}{T}\right) + \frac{T_c^4}{12T^3} \underline{M^4}$$





$$\frac{\partial f}{\partial M} = 0 \quad , \quad T_c M\left(1 - \frac{T_c}{T}\right) + \frac{T_c^{\,4}}{3T^3} M^3 = 0$$

$$M^2 = 3\left(\frac{T}{T_c}\right)^3\left(\frac{T_c}{T} - 1\right)$$

$$= 3\left(\frac{T}{T_c}\right)^2\left(1 - \frac{T}{T_c}\right)$$

$$M = \pm \frac{T}{T_c}\sqrt{3\left(1 - \frac{T}{T_c}\right)}$$

so that very near T_c

$$M \sim \left(T_c - T\right)^{\beta}$$

, where $\boxed{\beta = \frac{1}{2}}$

MF Hamiltonian: $$H = -mJ\sum_i \sigma_i + \frac{1}{2}NJm^2 - B\sum_i \sigma_i$$

$$\Rightarrow F = \frac{NJm^2}{2} - NT\ln\left[2\cosh\left(\frac{mJ+B}{T}\right)\right]$$

$$M = \tanh\left(\frac{mJ+B}{T}\right)$$

χ

1) $T > T_c$: Assume M and B are "small"

$$M = \frac{MJ + B}{T} \Rightarrow M\left(1 - \frac{T_c}{T}\right) = \frac{B}{T}$$

$$\chi = \frac{\frac{1}{T}}{\left(1 - \frac{T_c}{T}\right)} = \frac{1}{T - T_c} = |T - T_c|^{-\gamma} \qquad \boxed{\gamma = 1}^{\,MF}$$

C_+

2) $T < T_c$ assignment Q 1