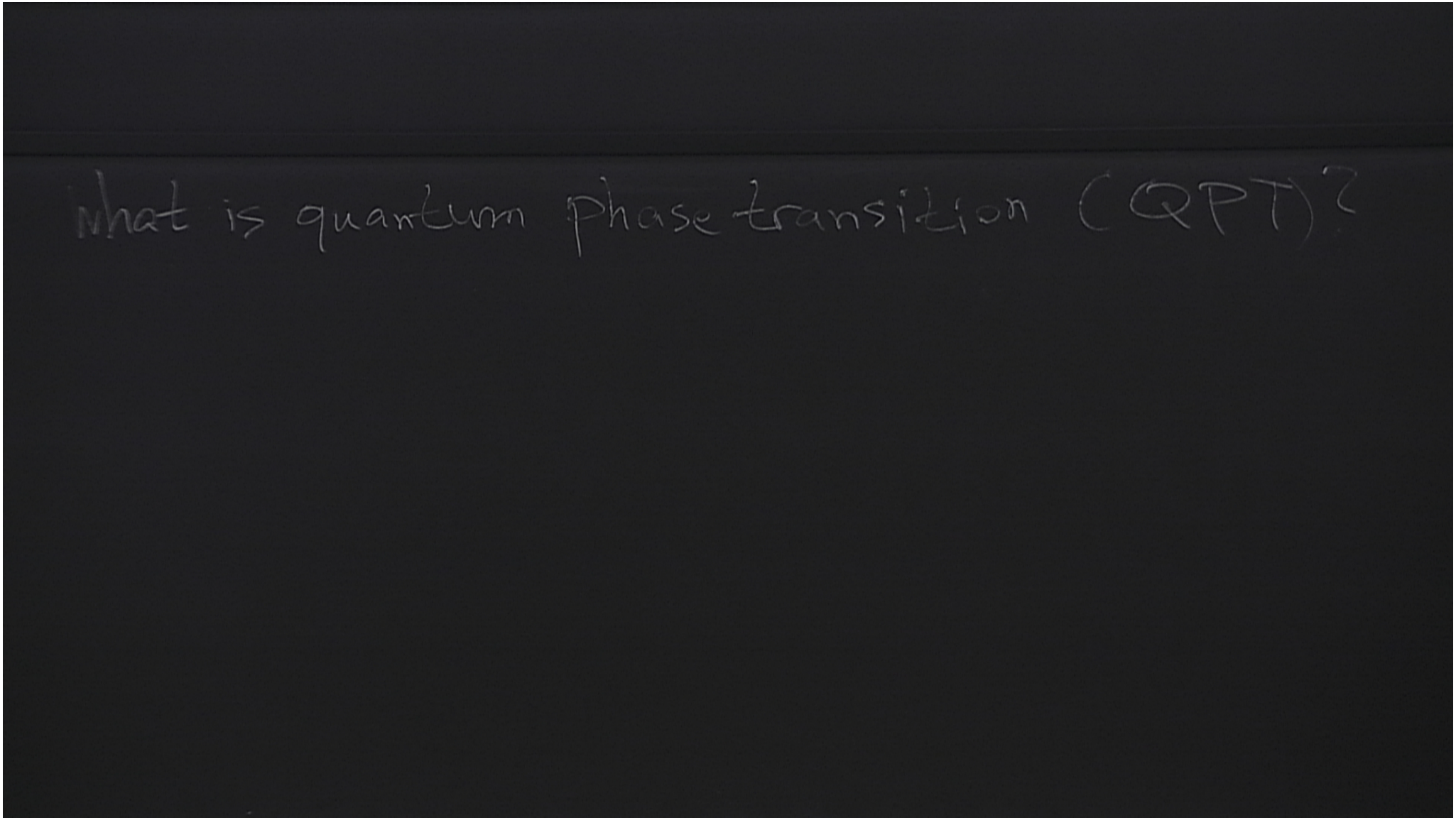
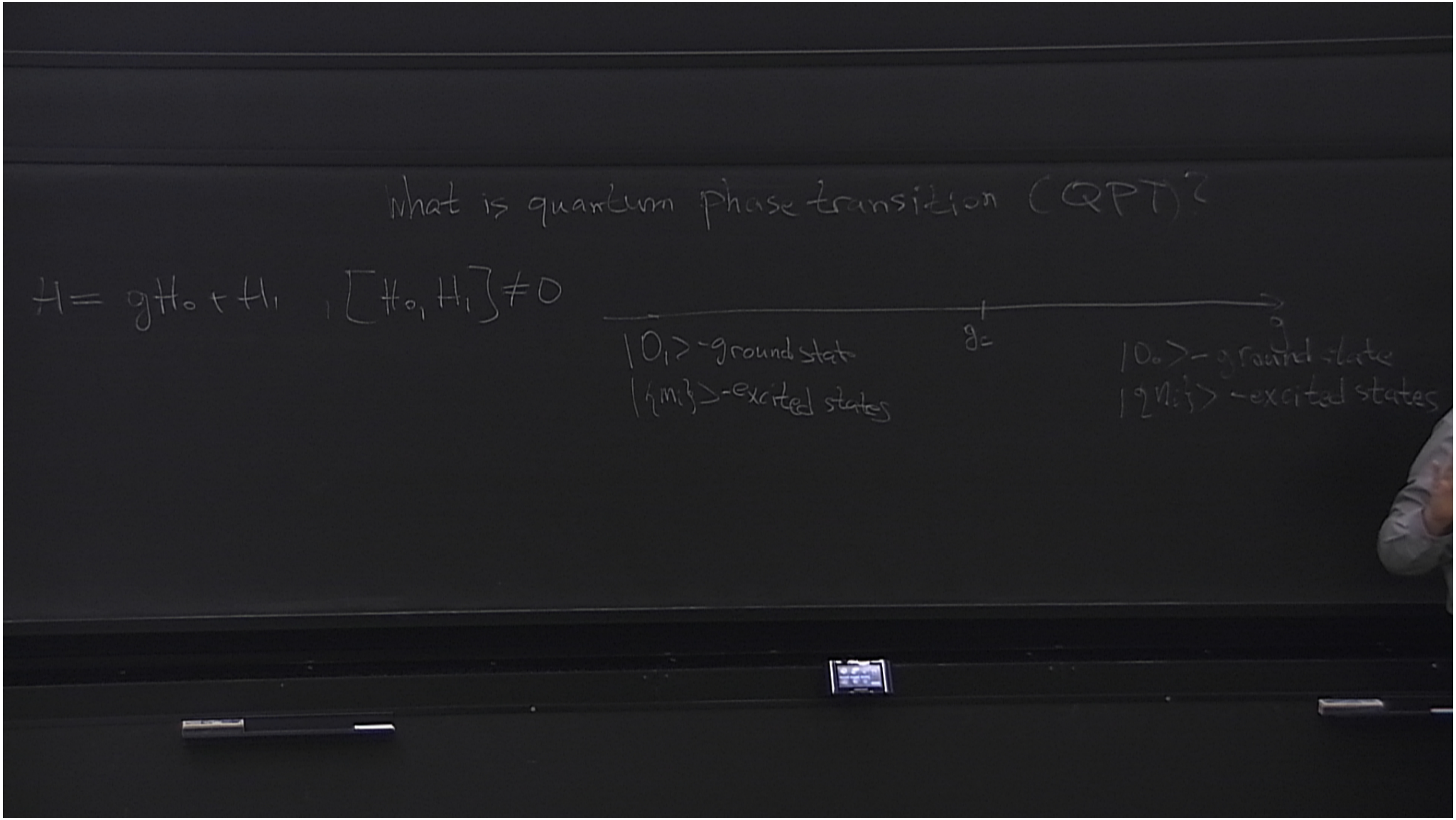
Title: PSI 2016/2017 Statistical Mechanics - Lecture 12

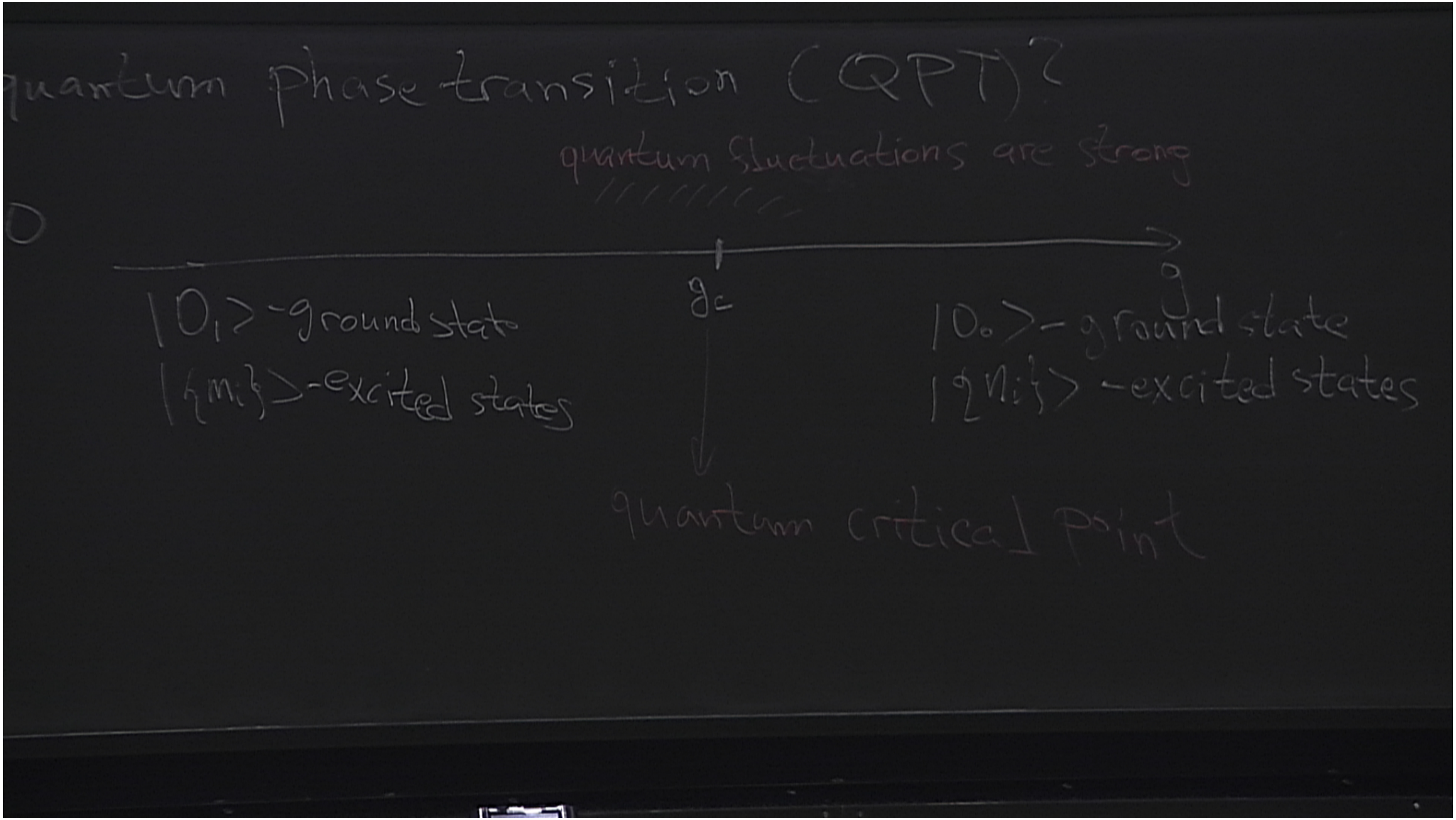
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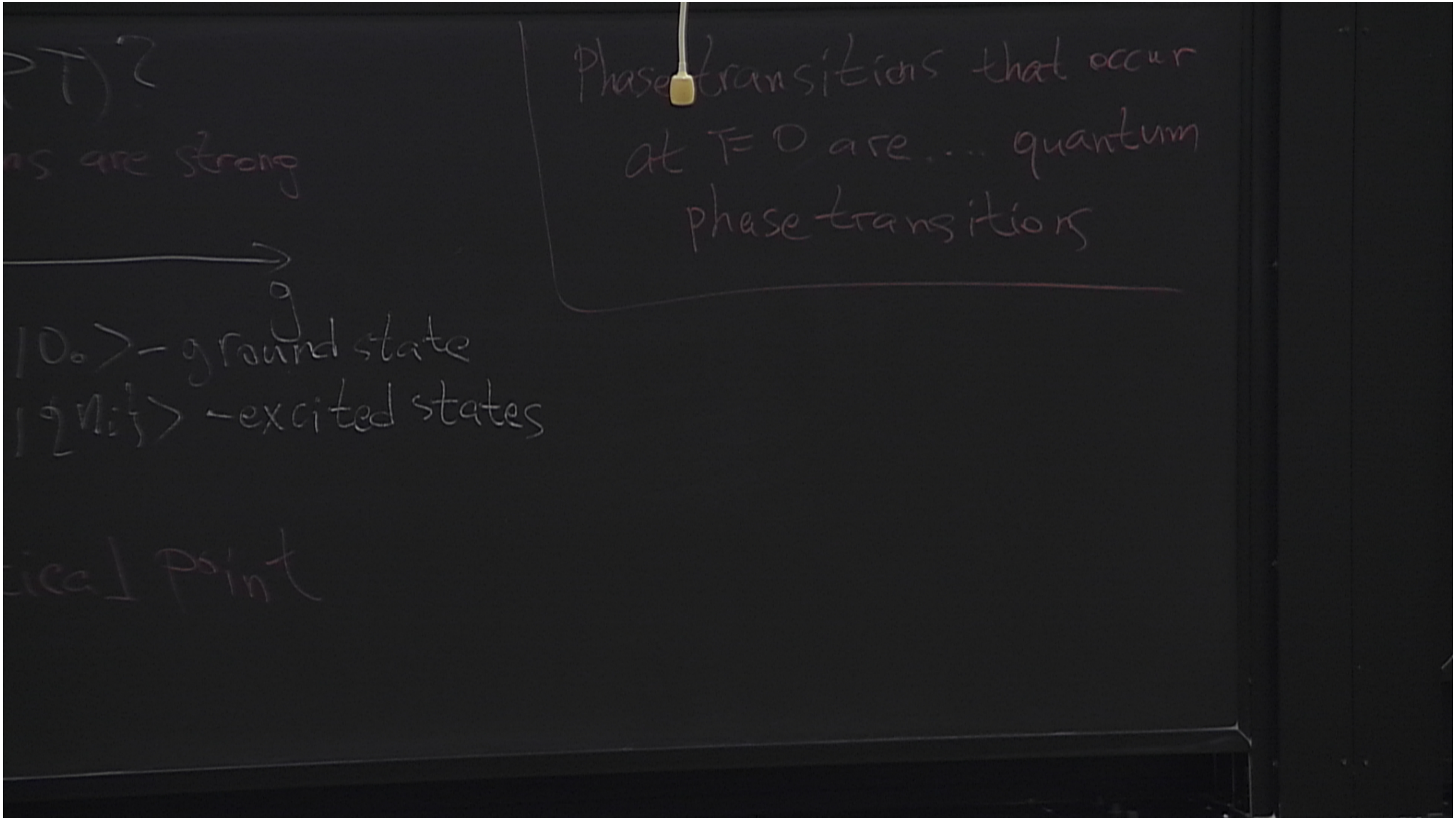
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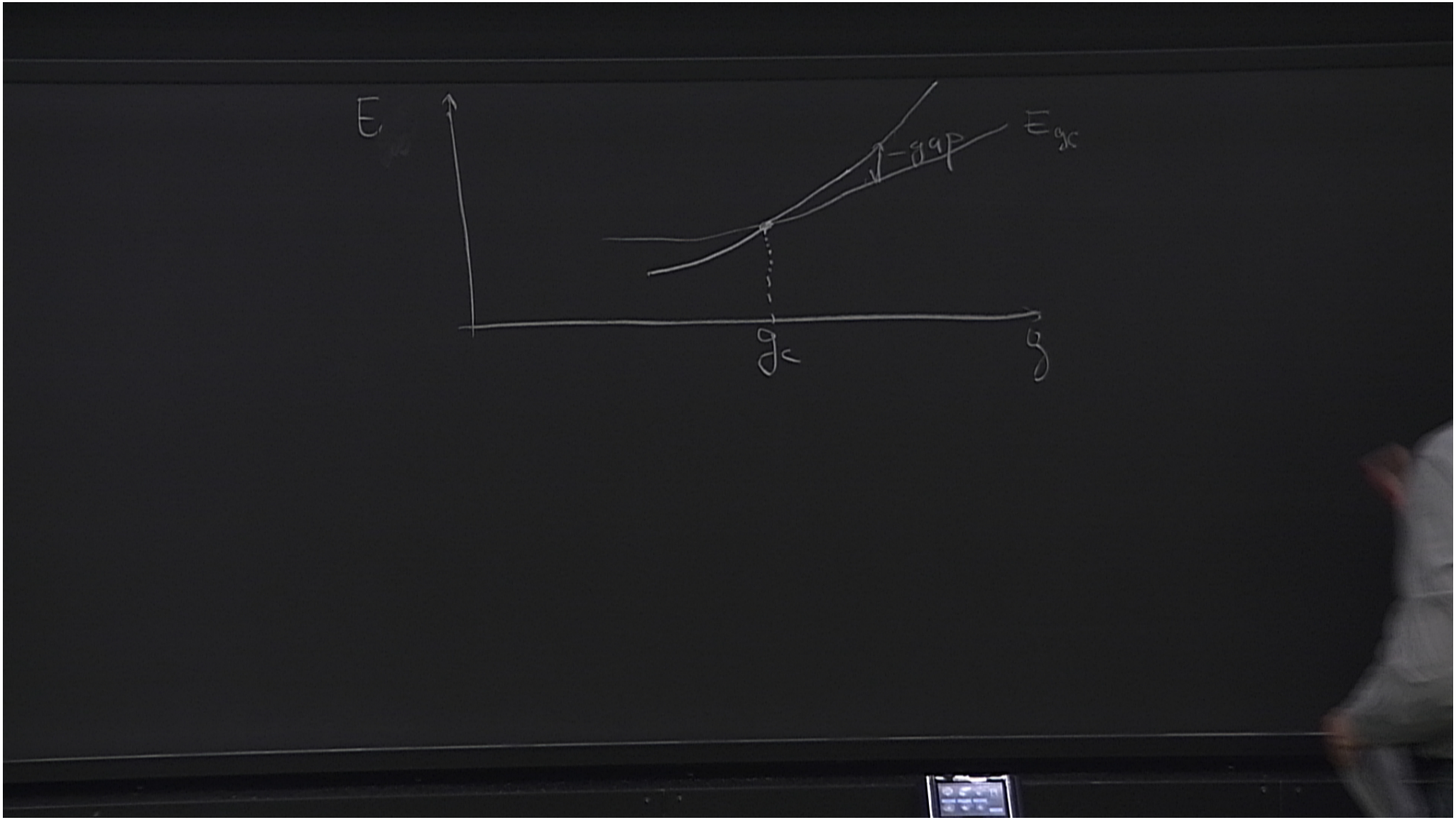
Abstract:

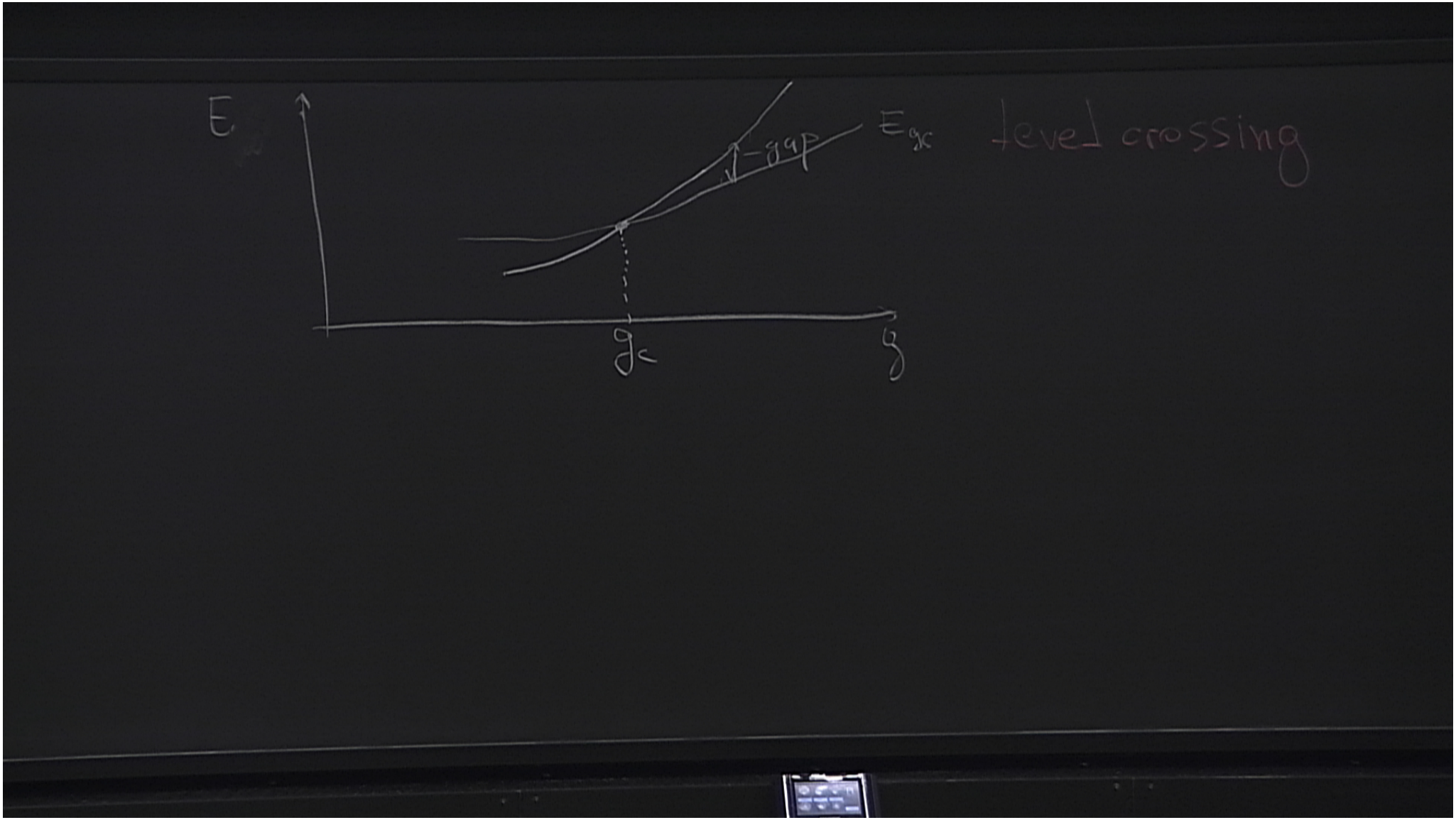

What is quantum phase transition (QPT)?

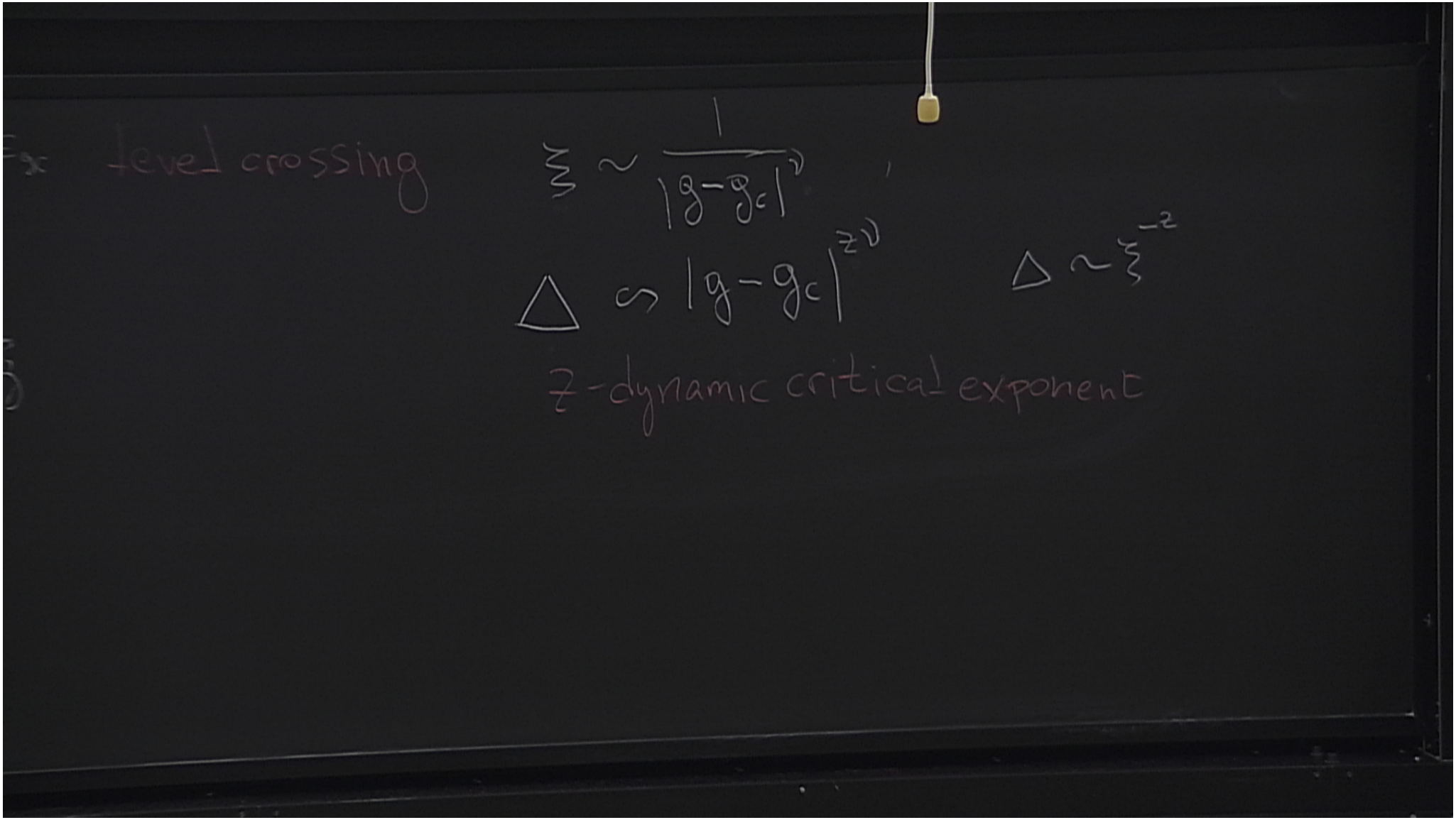

What is quantum phase transition (QPT)?
$H = gH_0 + H_1$, $[H_0, H_1] \neq 0$
g_c
$|0_1\rangle$ - ground state
$|\{n_i\}\rangle$ - excited states
$|0_0\rangle$ - ground state
$|\{n_i\}\rangle$ - excited states

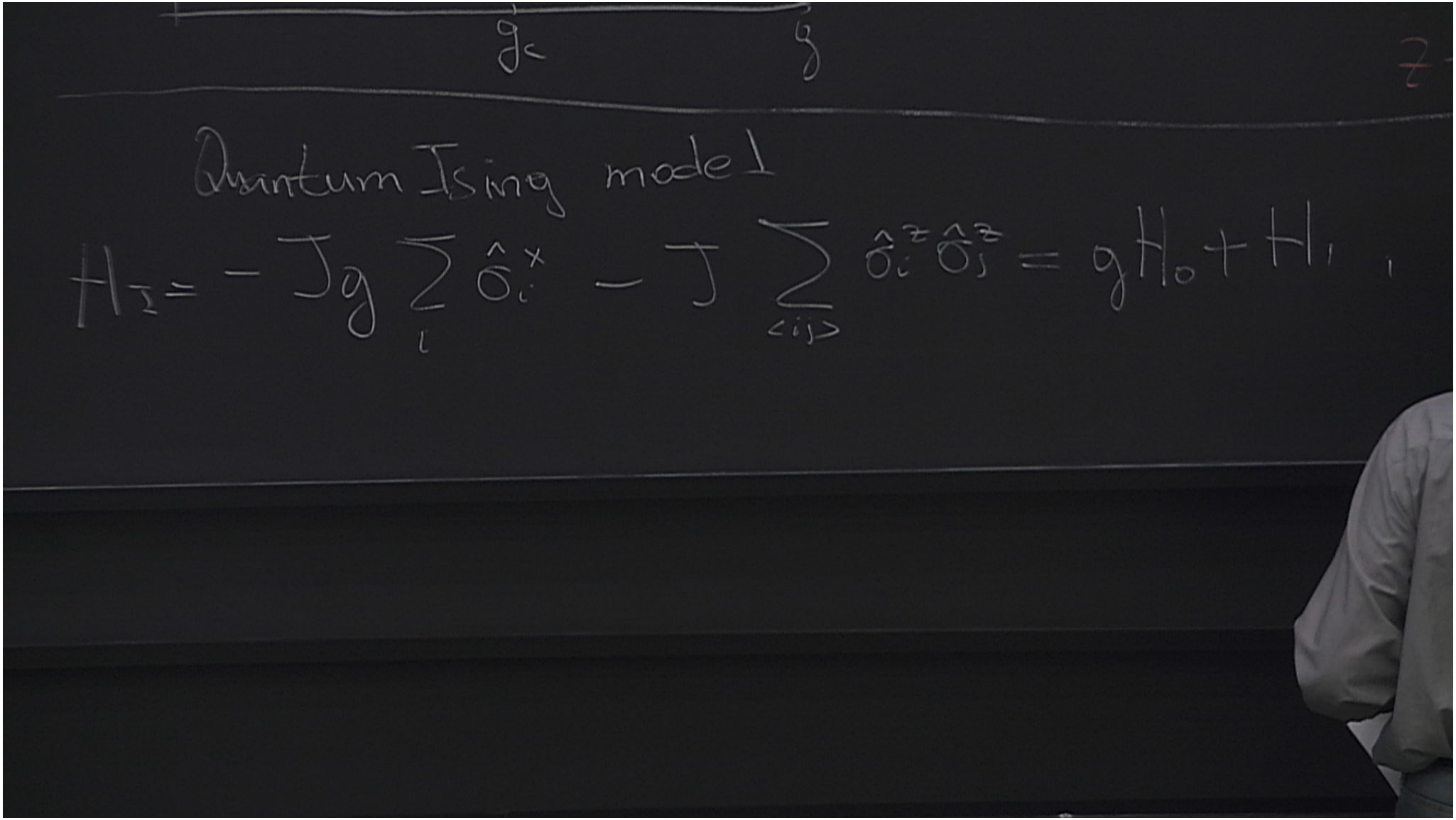

quantum phase transition (QPT)?
quantum fluctuations are strong
0
g
g_c
$|0_1\rangle$ - ground state
$|\{n_i\}\rangle$ - excited states
$|0_0\rangle$ - ground state
$|\{2n_i\}\rangle$ - excited states
quantum critical point

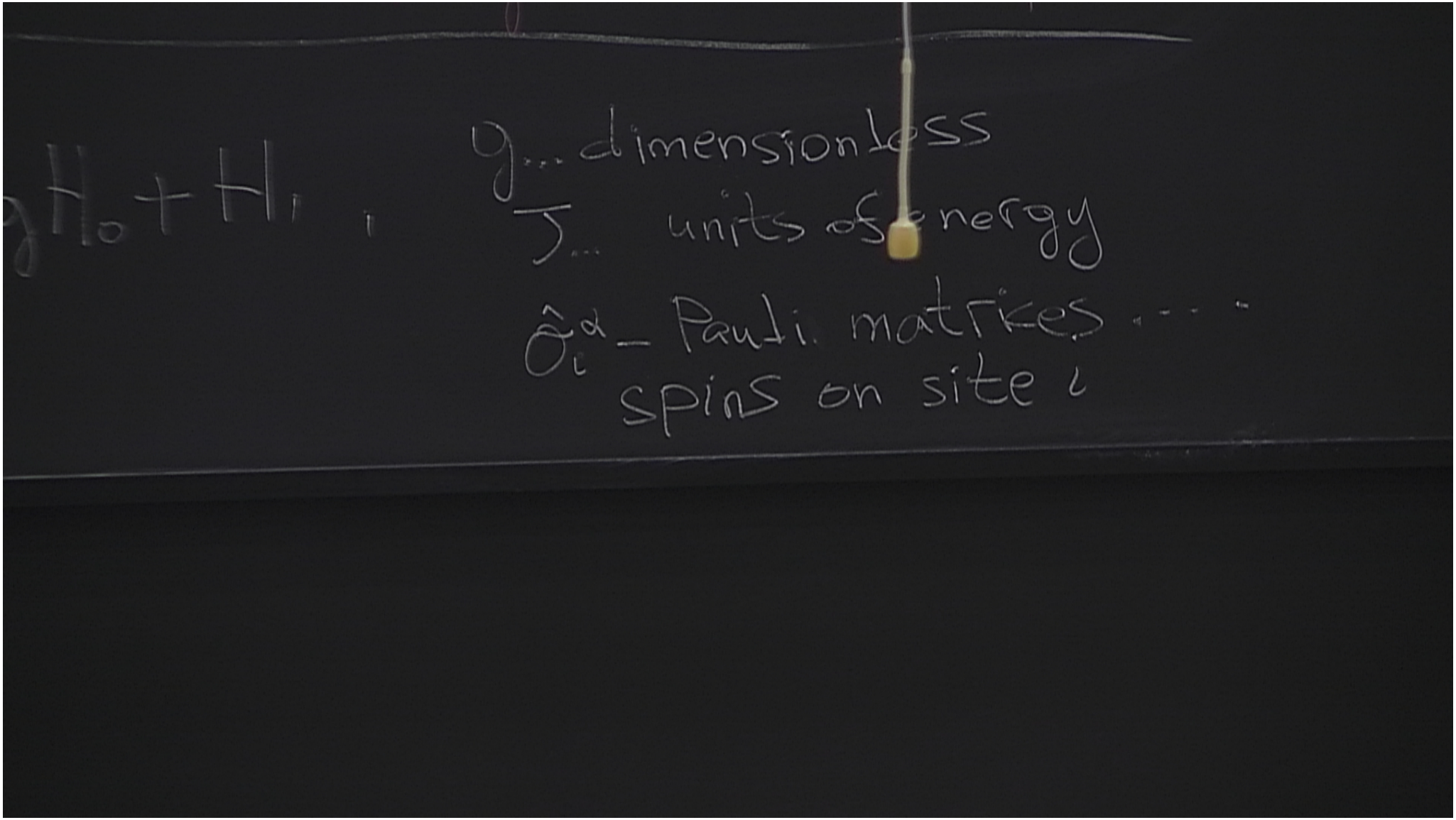

Phase transitions that occur at T=0 are... quantum phase transitions
|0₀⟩ - ground state
|2Nᵢ⟩ - excited states

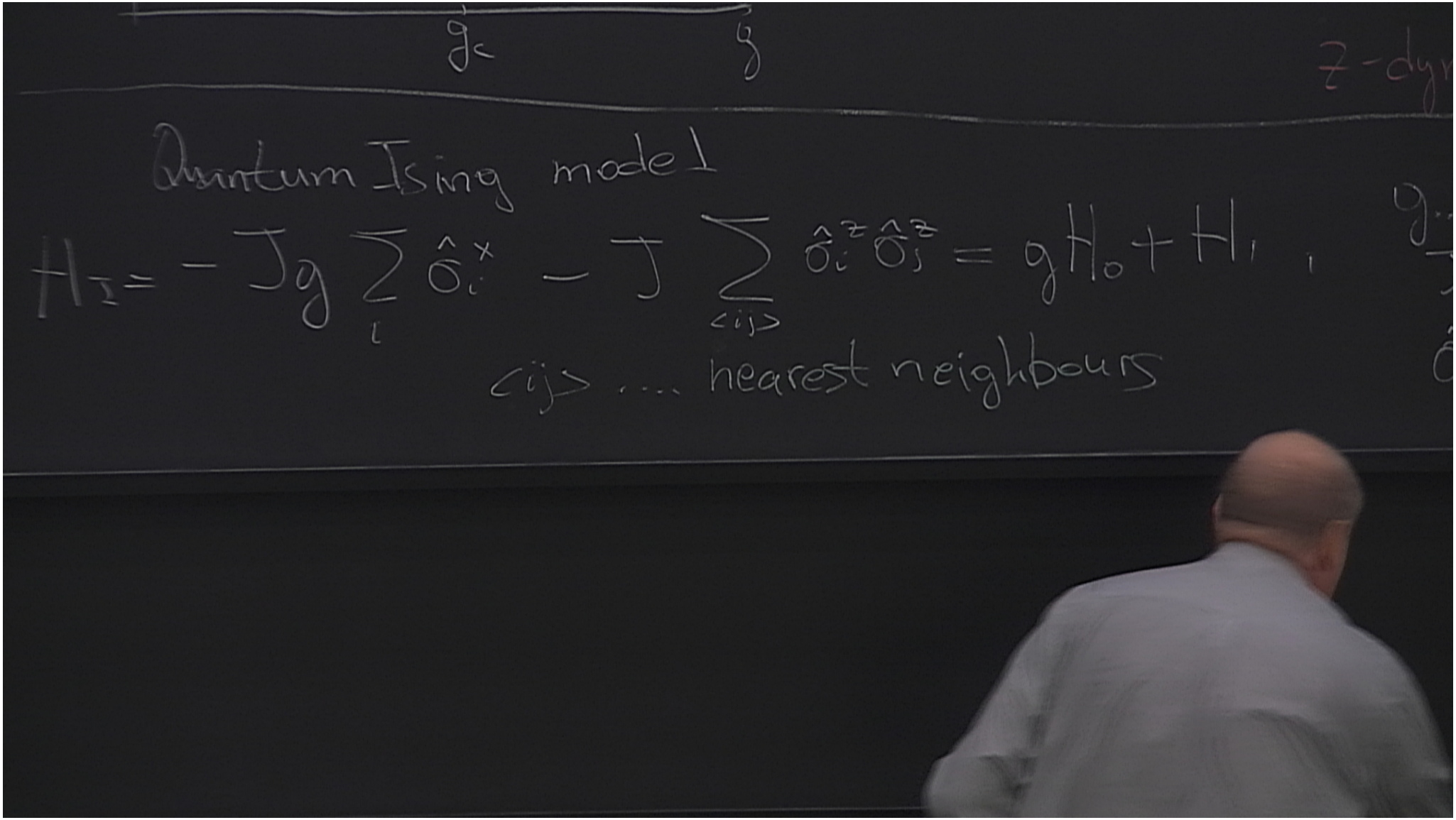

E
E_{gc}
$\sqrt{-gq}$
g_c
g

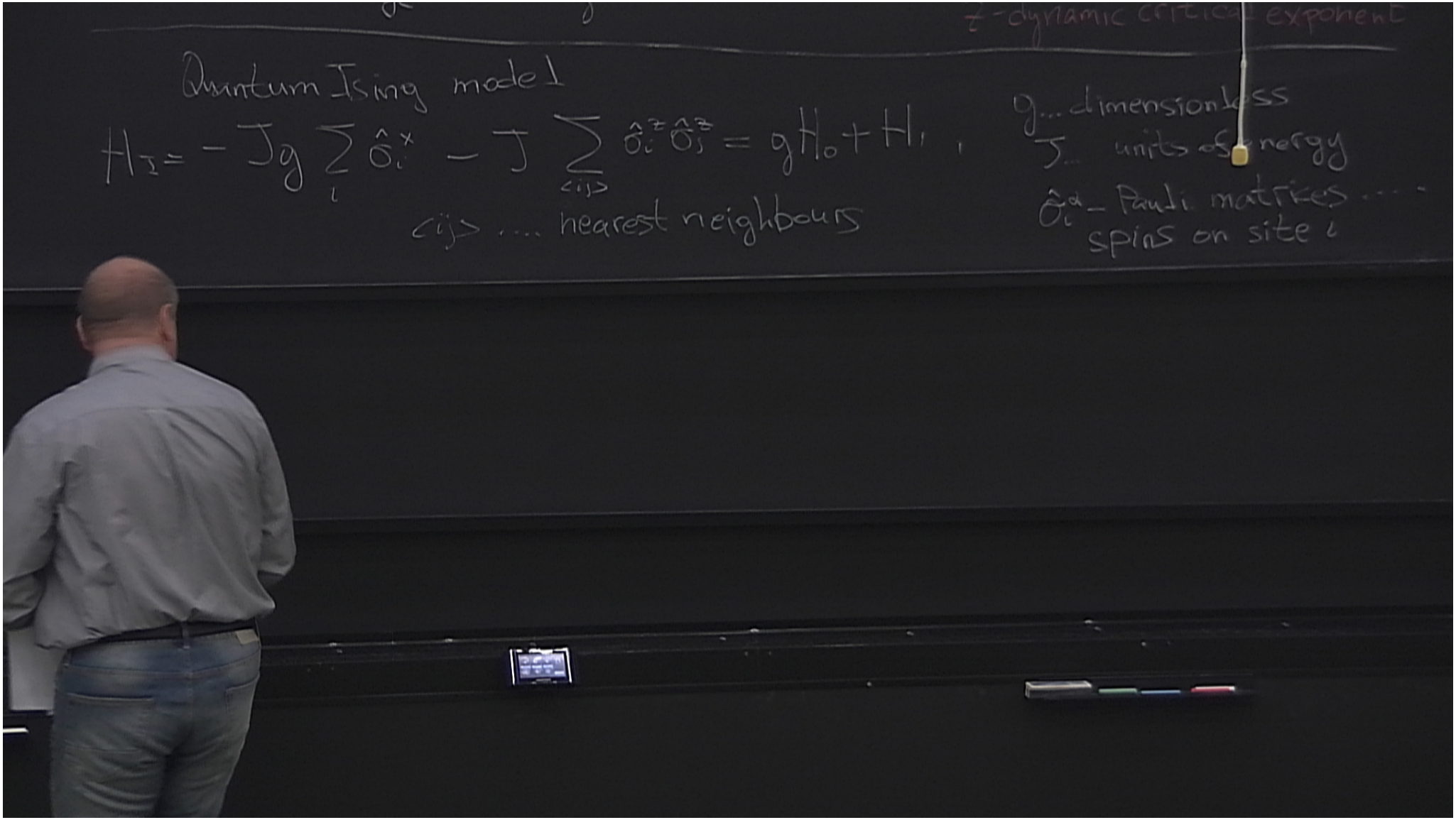

E
gap
E_{gs}
level crossing
g_c
g

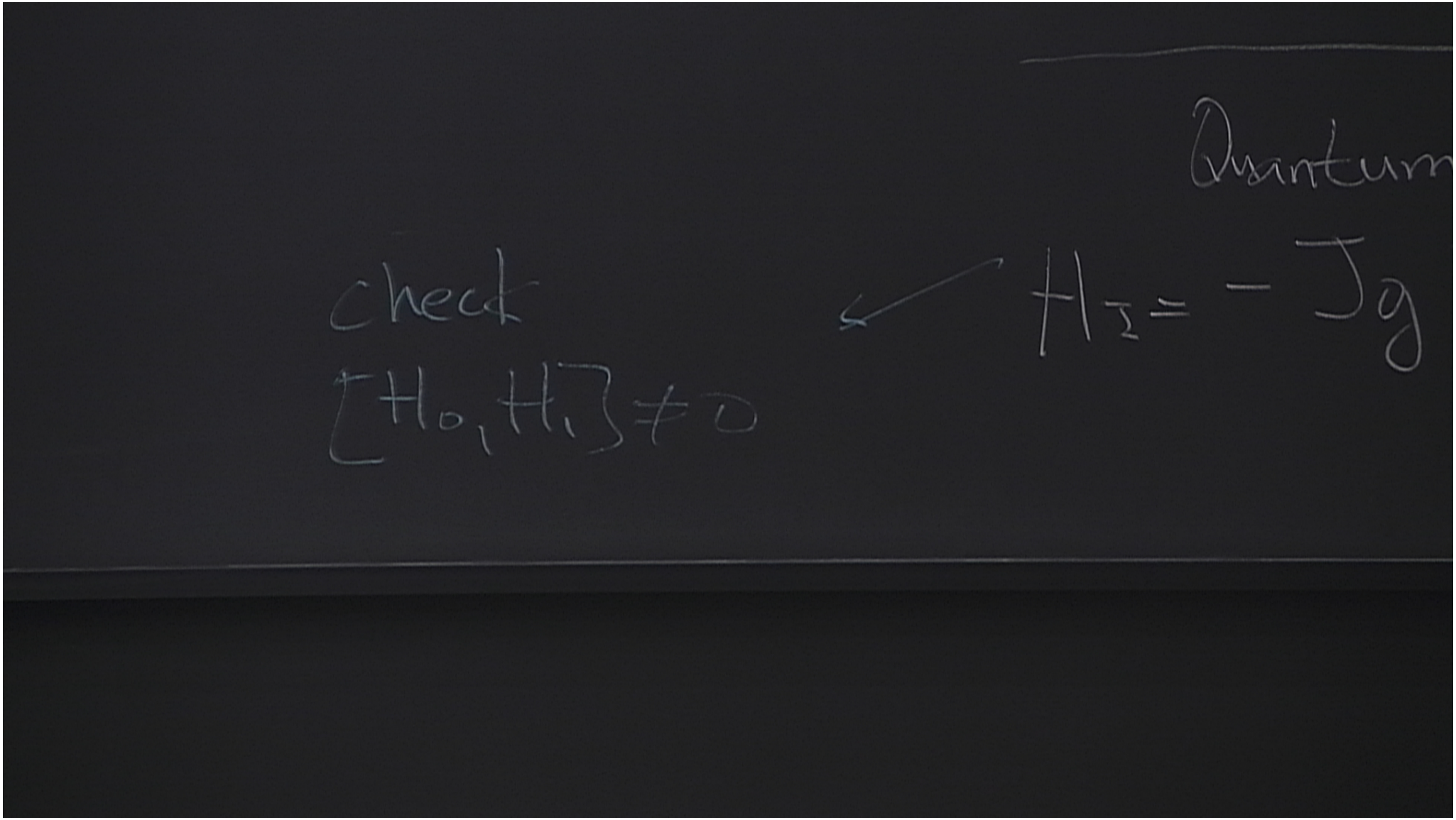

Ex level crossing
$\xi \sim \frac{1}{|g-g_c|^{\nu}}$
$\Delta \sim |g-g_c|^{z\nu}$
$\Delta \sim \xi^{-z}$
z-dynamic critical exponent

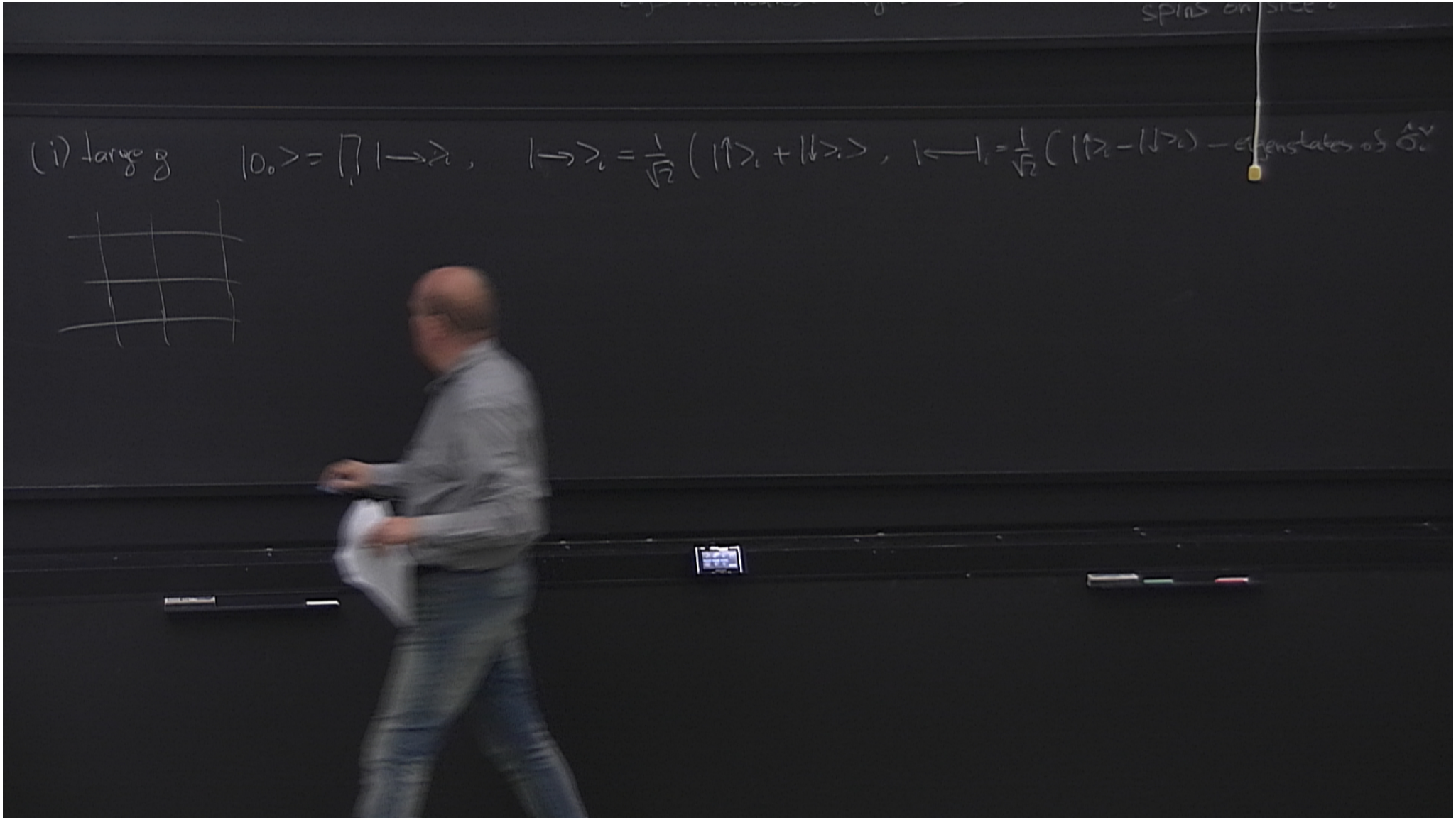

g<
g
Quantum Ising model
$H_I = -Jg\sum_i \hat{\sigma}_i^x - J\sum_{\langle ij\rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z = gH_0 + H_1$


$H_0 + H_1$;
g... dimensionless
J... units of energy
$\hat{\sigma}_i^\alpha$ - Pauli matrices ....
spins on site i

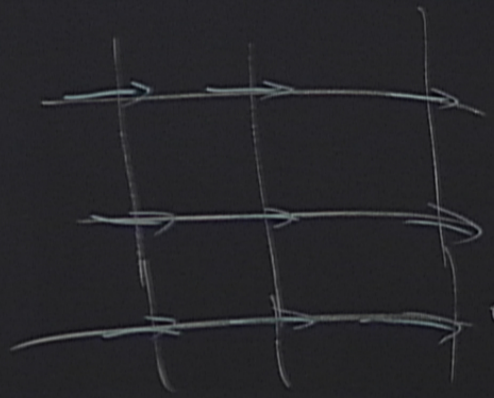

Quantum Ising model
$H_I = -Jg\sum_i \hat{\sigma}_i^x - J\sum_{\langle ij\rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z = gH_0 + H_1$,
$\langle ij\rangle$ .... nearest neighbours


z-dynamic critical exponent
Quantum Ising model
$H_I = -Jg\sum_i \hat{\sigma}_i^x - J\sum_{\langle ij\rangle} \hat{\sigma}_i^z\hat{\sigma}_j^z = gH_0 + H_1$
g... dimensionless
J... units of energy
$\hat{\sigma}_i^\alpha$ - Pauli matrices ... spins on site i
$\langle ij\rangle$ ... nearest neighbours


Quantum
check
$H_\Sigma = -J_g$
$[H_0, H_1] \neq 0$


(i) large g
$|0_0\rangle = \prod_i |\rightarrow\rangle_i$,
$|\rightarrow\rangle_i = \frac{1}{\sqrt{2}}(|\uparrow\rangle_i + |\downarrow\rangle_i)$,
$|\leftarrow\rangle_i = \frac{1}{\sqrt{2}}(|\uparrow\rangle_i - |\downarrow\rangle_i)$ – eigenstates of $\hat{\sigma}^x_i$

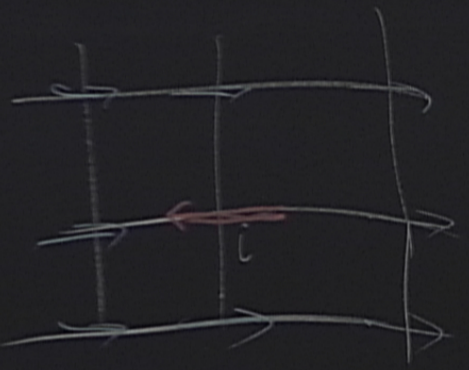
(i) large g $\quad |0_0\rangle = \prod_i |\rightarrow\rangle_i , \quad |\rightarrow\rangle_i =$



$E_{gs} = -NJg$

← ground state

$|\rightarrow\rangle_i = \frac{1}{\sqrt{2}}(|\uparrow\rangle_i + |\downarrow\rangle_i)$, $|\leftarrow\rangle_i = \frac{1}{\sqrt{2}}(|\uparrow\rangle_i - |\downarrow\rangle_i)$ — eigenst



$$|i\rangle = |\leftarrow\rangle_i \prod_{j \neq i} |\rightarrow\rangle_j$$

$$E_1 = -NJ_g + 2J_g$$

First excited state / N excited states

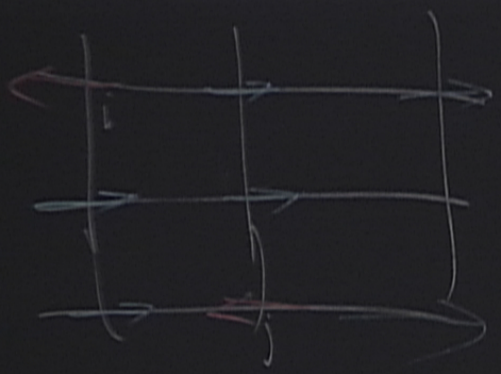
$|\rightarrow\rangle_i = \frac{1}{\sqrt{2}}(|\uparrow\rangle_i + |\downarrow\rangle_i)$, $|\leftarrow\rangle_i = \frac{1}{\sqrt{2}}(|\uparrow\rangle_i - |\downarrow\rangle_i)$ — eigenstates



$$|i\rangle = |\leftarrow\rangle_i \prod_{j \neq i} |\rightarrow\rangle_j$$

$$E_1 = -NJ_g + 2J_g$$

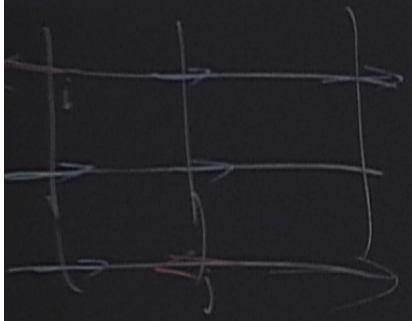
First excited state (N excited states) — "one-particle" states



$|i,j\rangle = |\leftarrow_i \leftarrow_j \prod_{h\neq i,j} |\rightarrow\rangle_n$

$E_2 = -NJ_g + 4J_g$ ... second excited states

$\left(\frac{N(N-1)}{2}\right.$ of such states)



$|i,j\rangle = |\leftarrow_i\rangle_i |\leftarrow_j\rangle_j \prod_{h\neq i,j} |\rightarrow\rangle_h$

$E_2 = -NJ_g + 4J_g$ ... second excited states - "two-particle" states

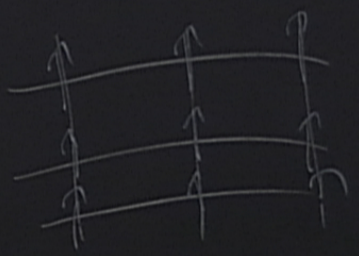
$\left(\frac{N(N-1)}{2}\right)$ of such states)

also p-particle states $\left(\frac{N!}{p!(N-p)!}\right)$ have energy $E_g + 2pJ_g$

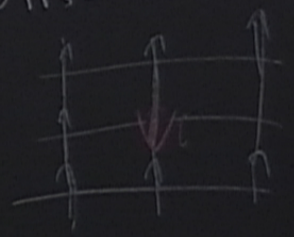
(ii) large g. $|0_1\rangle = \prod_i |\uparrow\rangle_i$ or $|0_1\rangle = \prod_i |\downarrow\rangle_i$

$M^z = \langle 0_1 | \hat{\sigma}_i^z | 0_1 \rangle = 1$

$E_{gs} = -NJd$

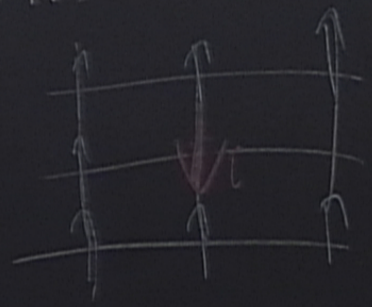


$\Rightarrow$ first excited state



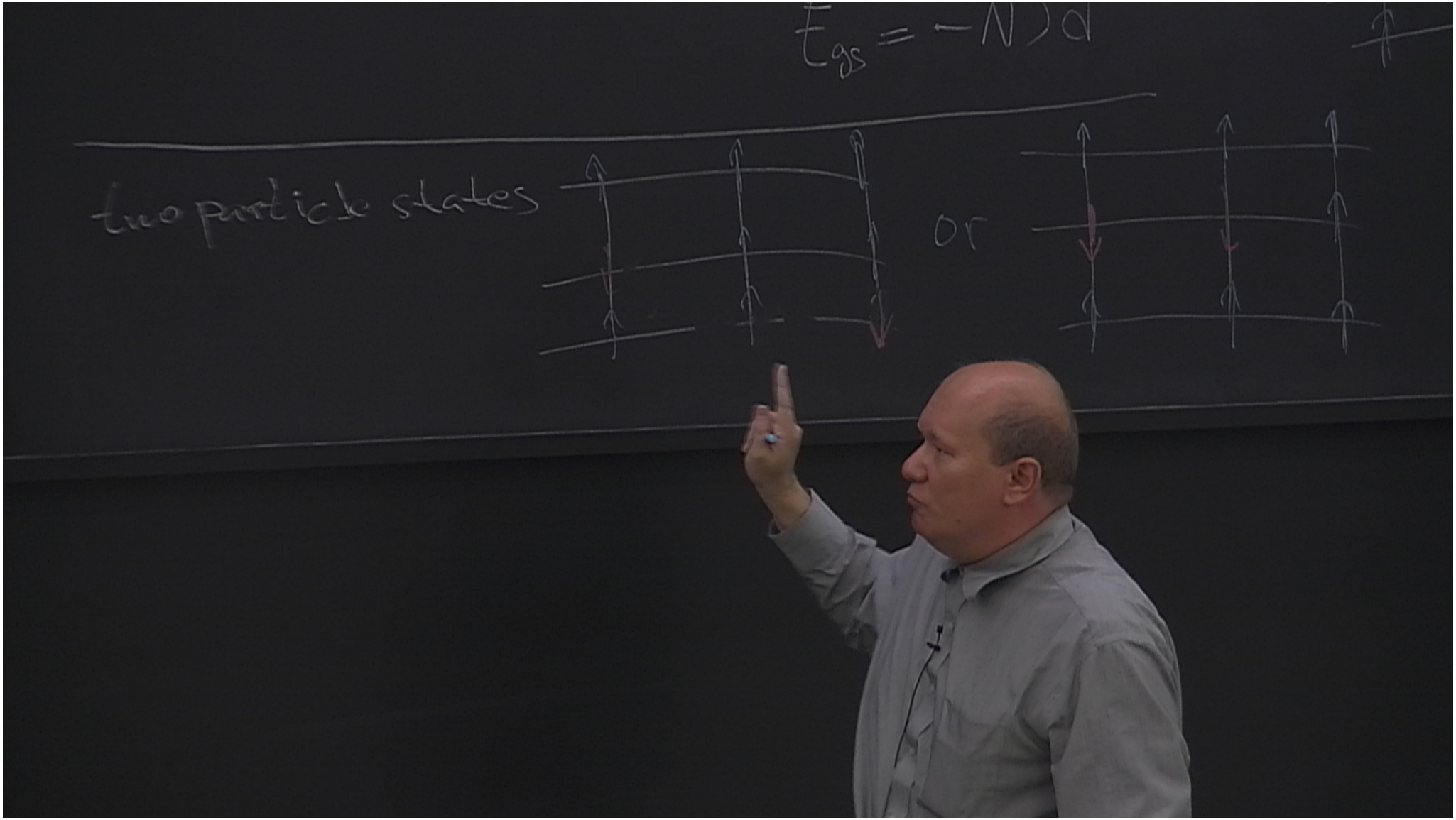
$|\uparrow\rangle_z$

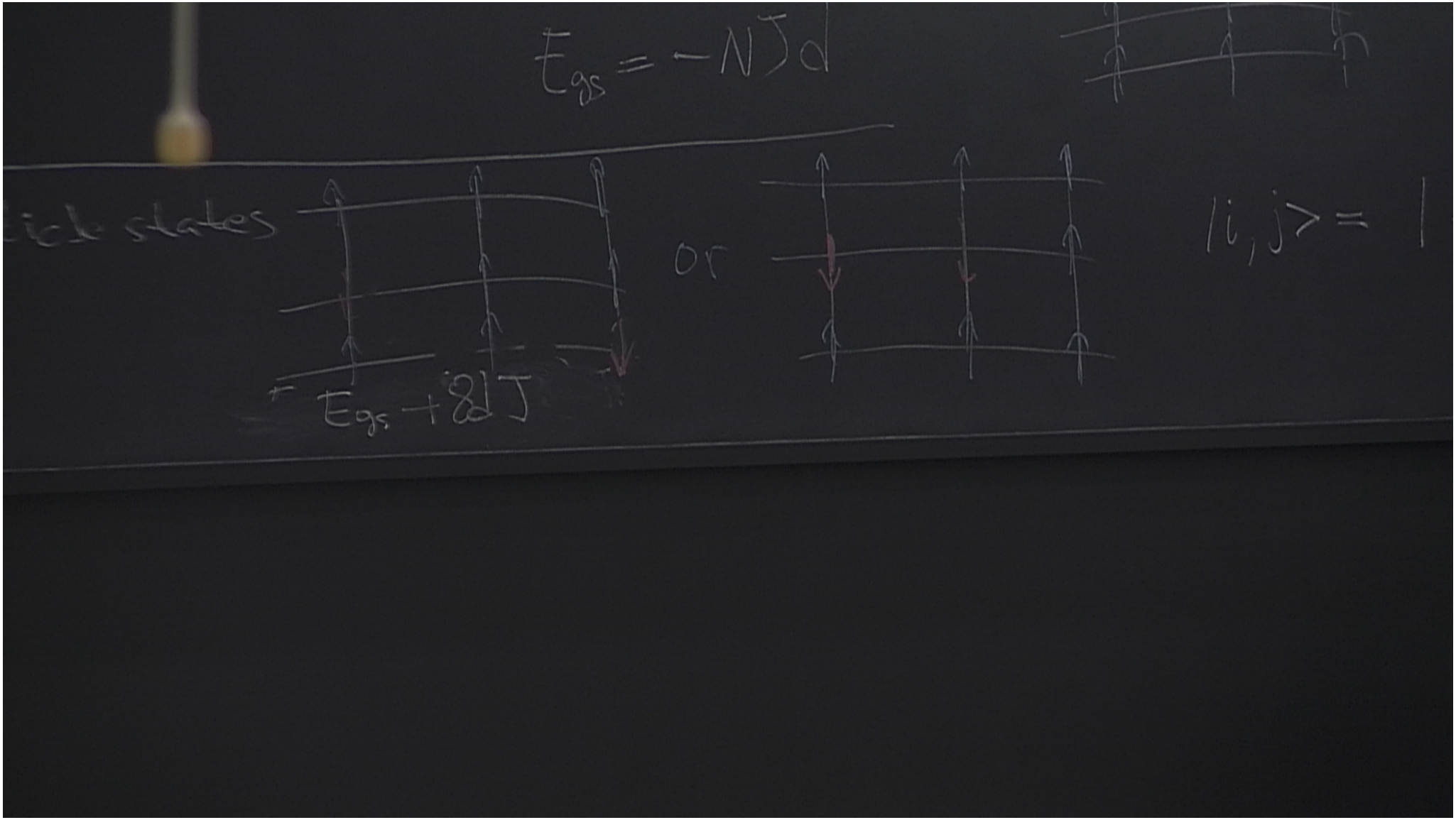
$\Rightarrow$ first excited state

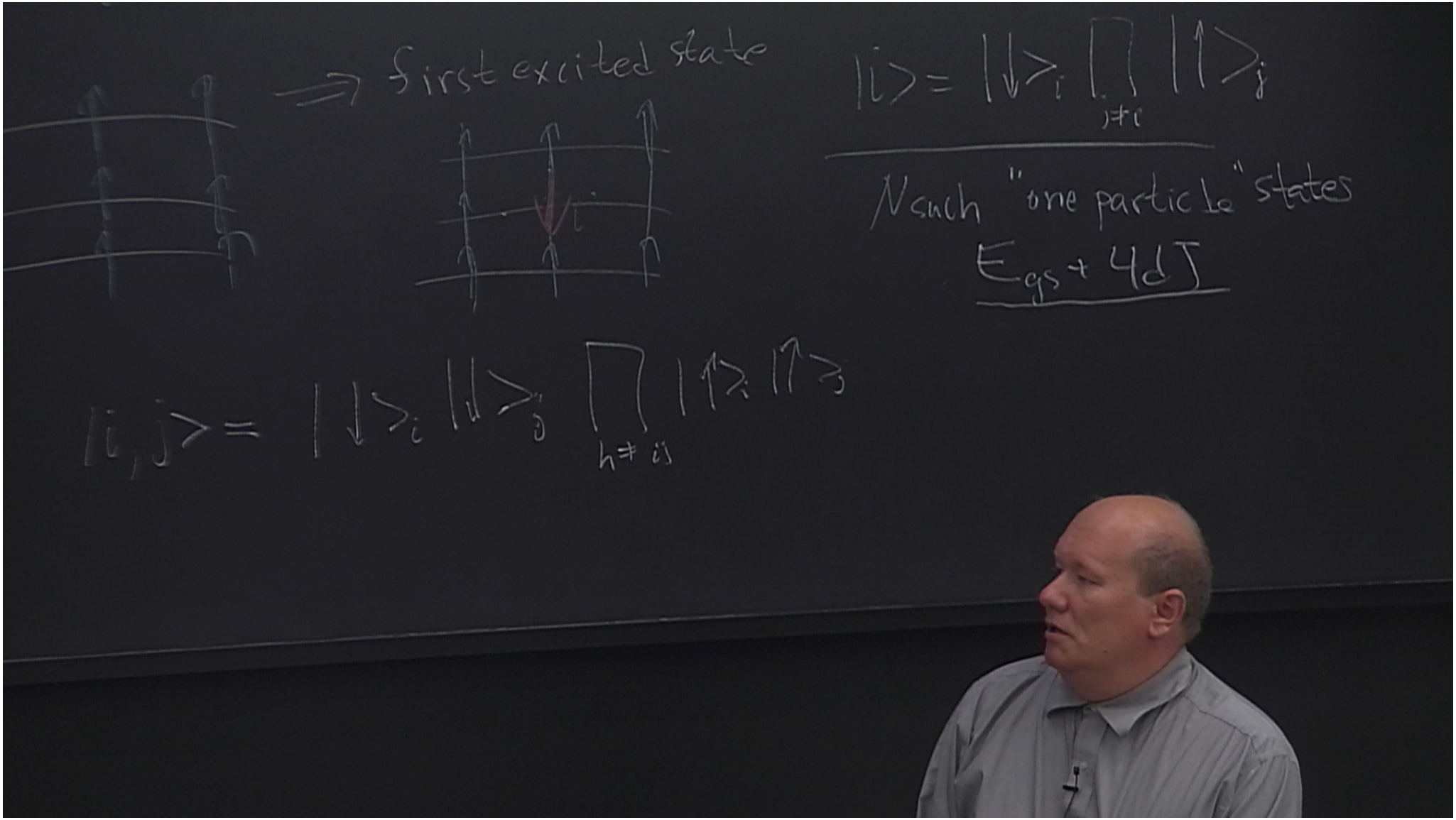


$|i\rangle = |\downarrow\rangle_i \prod_{j \neq i} |\uparrow\rangle_j$

N such "one particle" states


two particle states
or

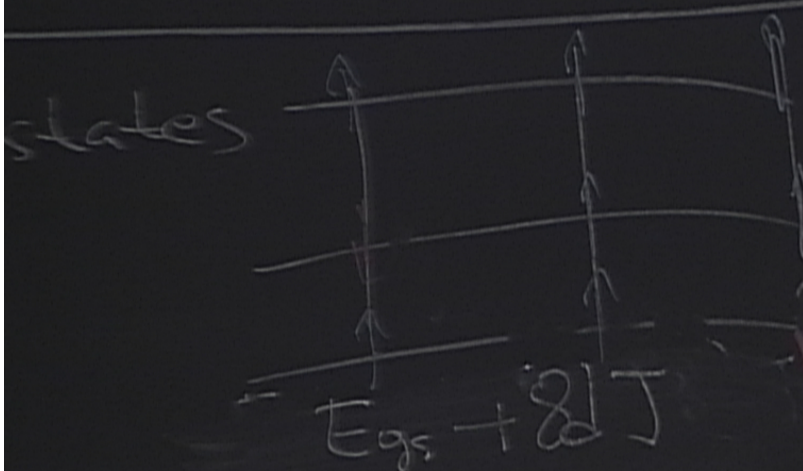

$E_{gs} = -NJ\alpha$
tick states
or
$|i,j\rangle =$
$E_{gs} + 8\alpha J$


⇒ first excited state
$|i\rangle = |\downarrow\rangle_i \prod_{j\neq i} |\uparrow\rangle_j$
N such "one particle" states
$E_{gs} + 4dJ$
$|i,j\rangle = |\downarrow\rangle_i |\downarrow\rangle_j \prod_{k\neq ij} |\uparrow\rangle_k |\uparrow\rangle_j$

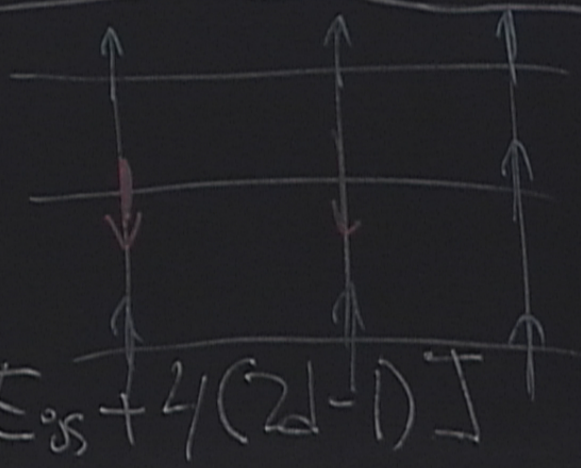
$M^z = \langle 0_i | \sigma_i^z | 0_i \rangle = 1$

$E_{gs} = -NJd$





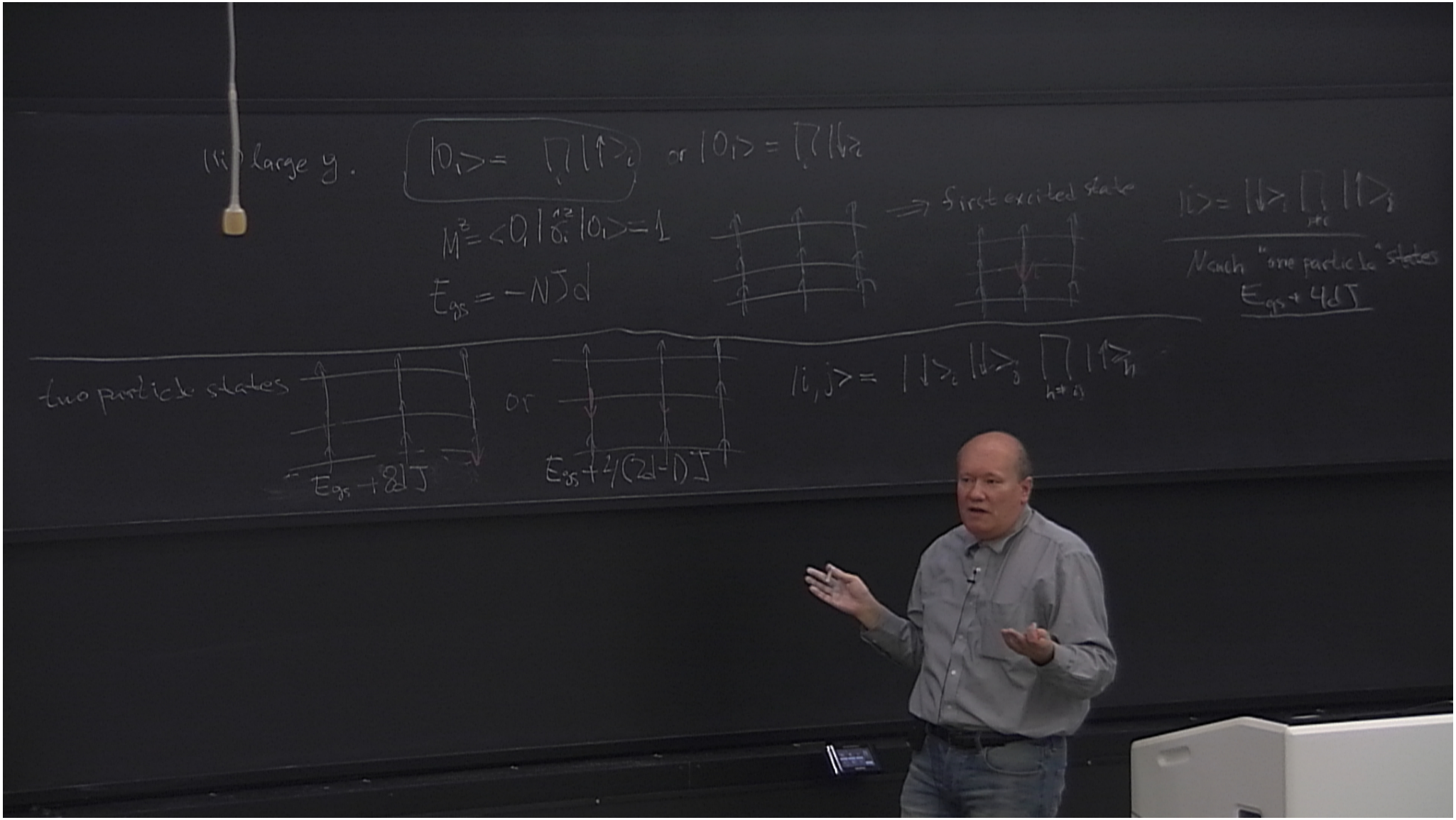
or

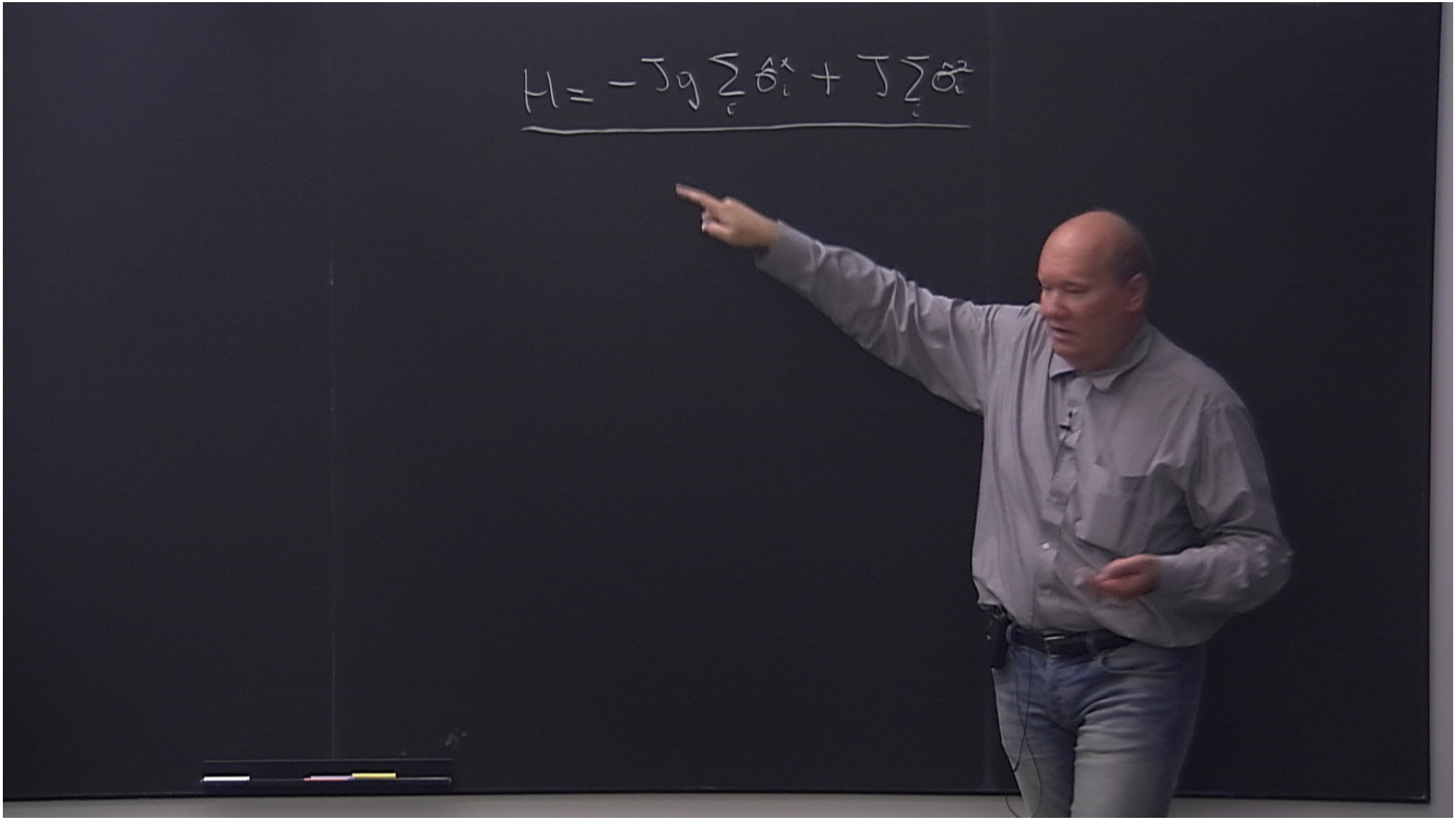


$|i,j\rangle =$

$E_{gs} + 2dJ$

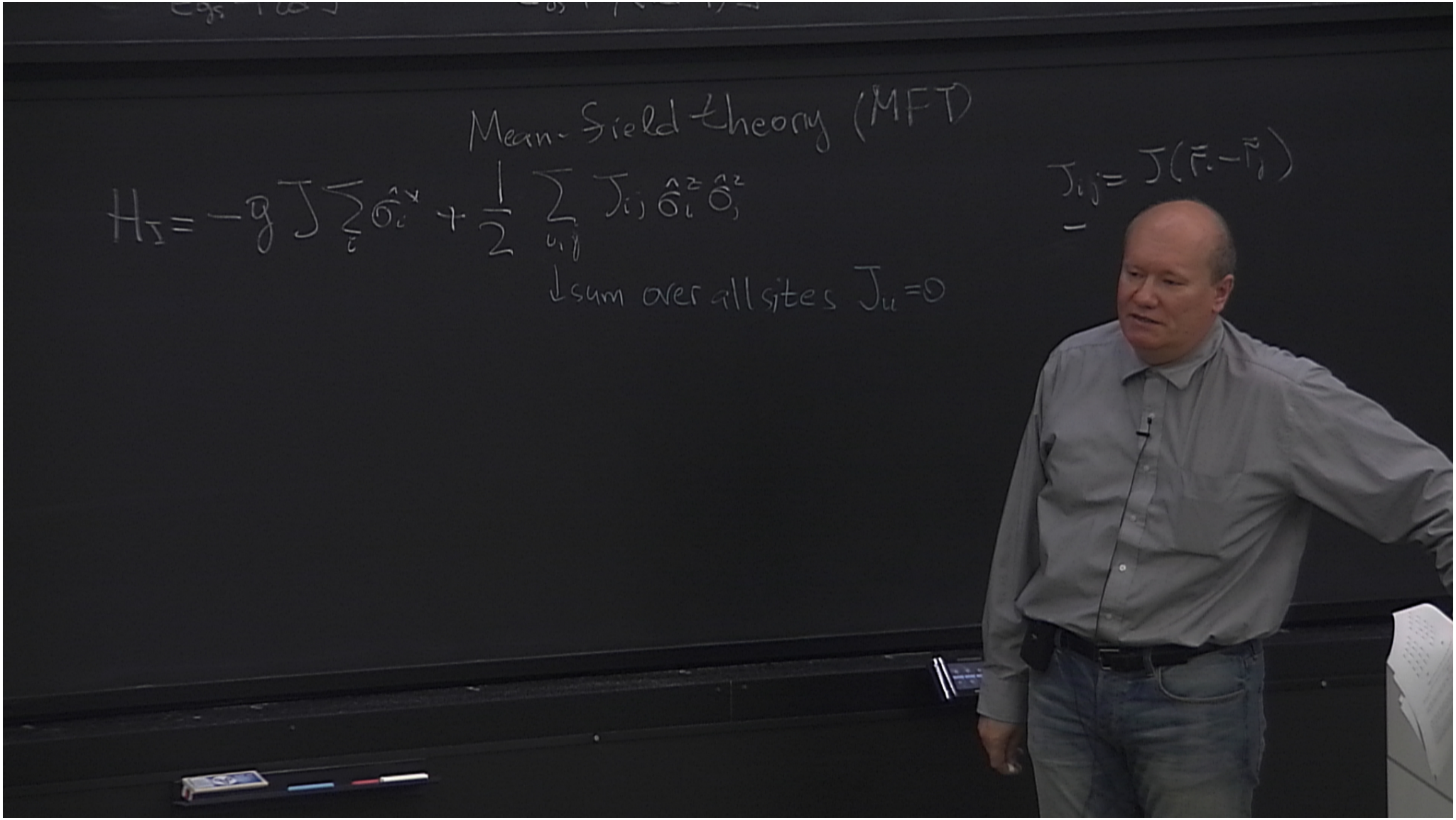
$E_{gs} + 4(2d-1)J$

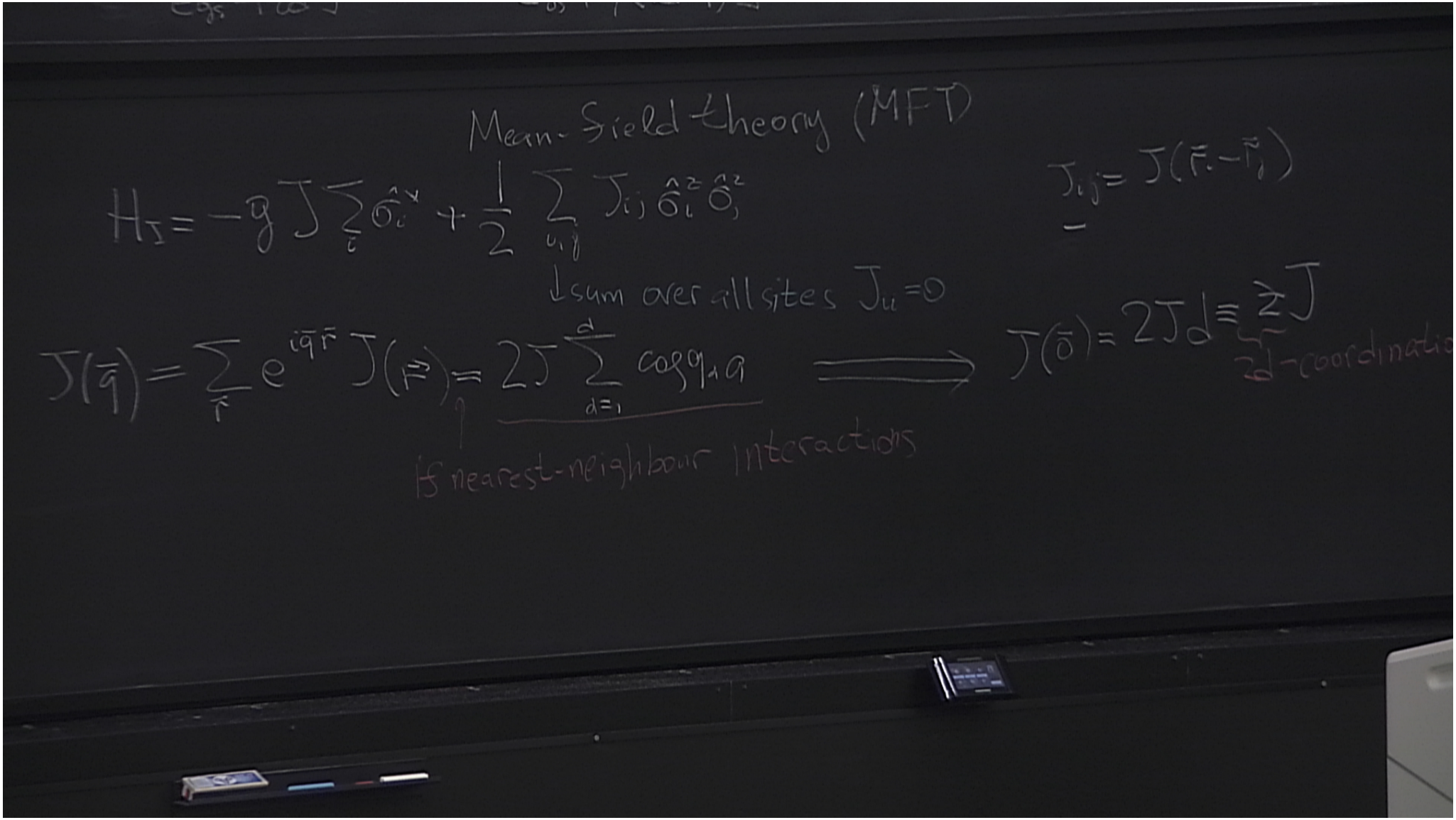

large y.
$|0_1\rangle = \prod_i |\uparrow\rangle_i$ or $|0_1\rangle = \prod_i |\downarrow\rangle_i$
$M^z = \langle 0_1 | \sum_i \sigma_i^z | 0_1 \rangle = 1$
$E_{gs} = -NJd$
⇒ first excited state
$|i\rangle = |\downarrow\rangle_i \prod_{n \neq i} |\uparrow\rangle_n$
N each "one particle" states
$E_{gs} + 4dJ$
two particle states
$E_{gs} + 2dJ$
or
$E_{gs} + 4(2d-1)J$
$|i,j\rangle = |\downarrow\rangle_i |\downarrow\rangle_j \prod_{n \neq i,j} |\uparrow\rangle_n$

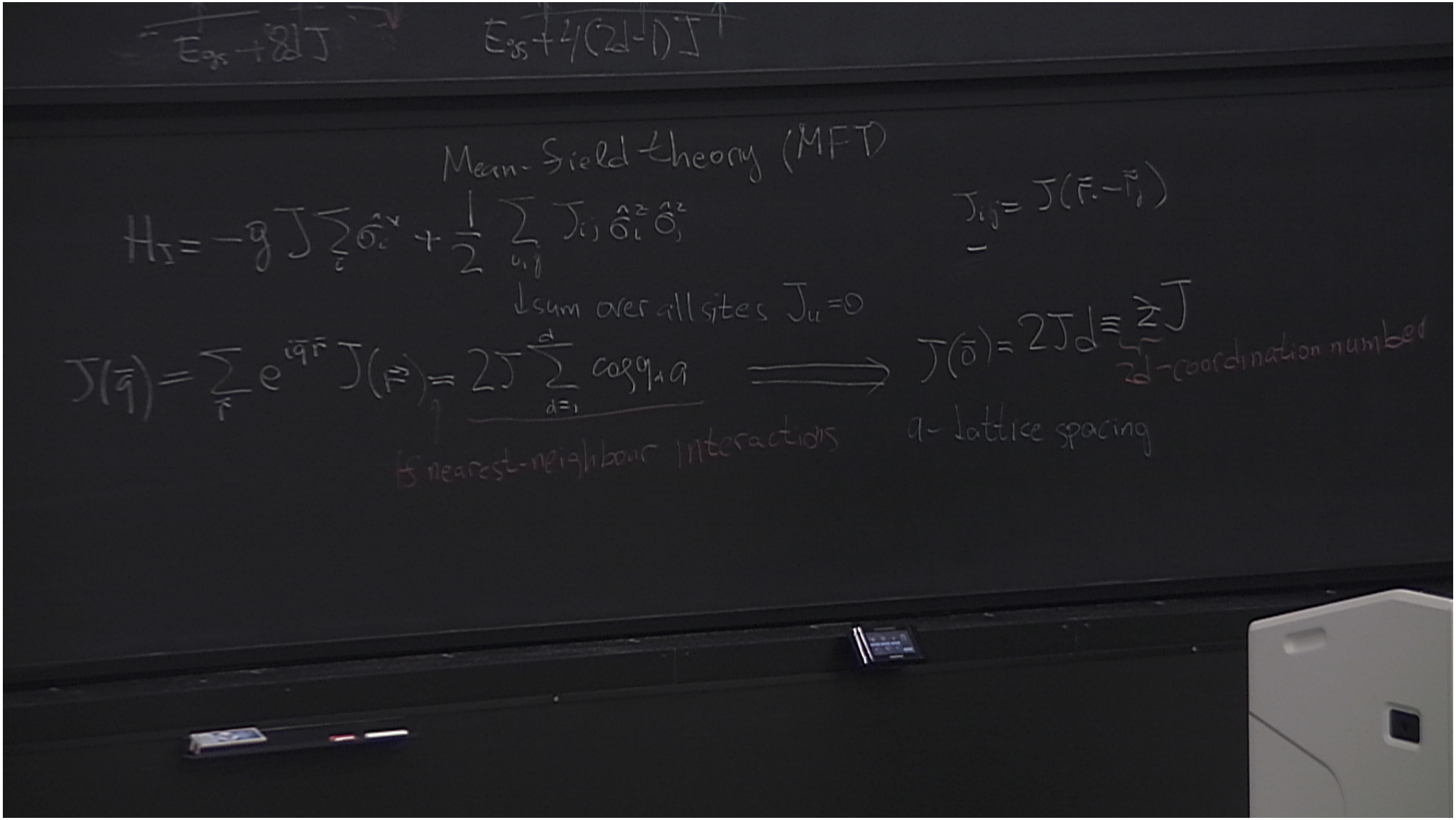

$H = -J_g \sum_i \hat{\sigma}_i^x + J \sum_i \hat{\sigma}_i^z$

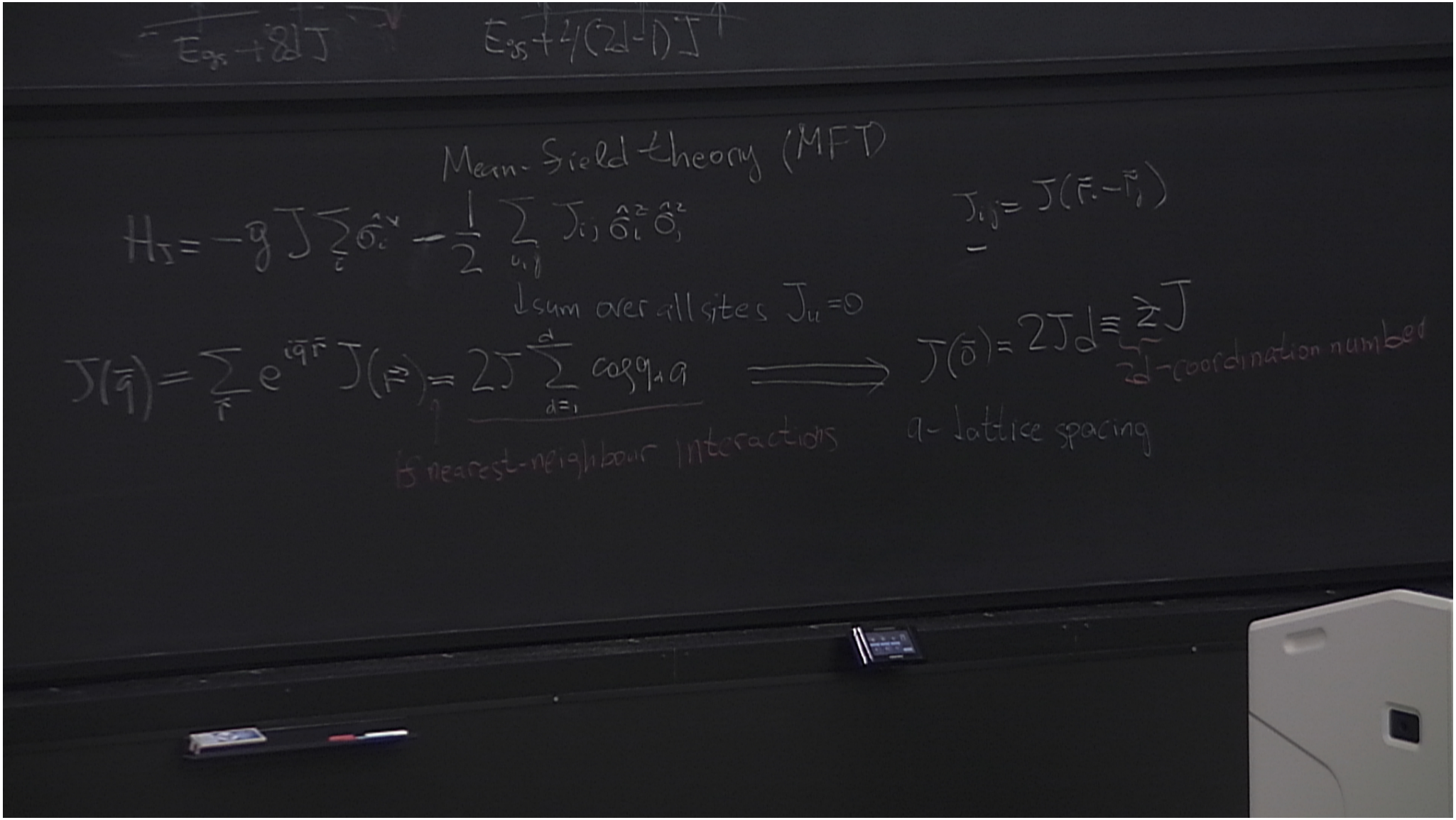
$$H = -J_g \sum_i \hat{\sigma}_i^x + J \sum_i \hat{\sigma}_i^z$$

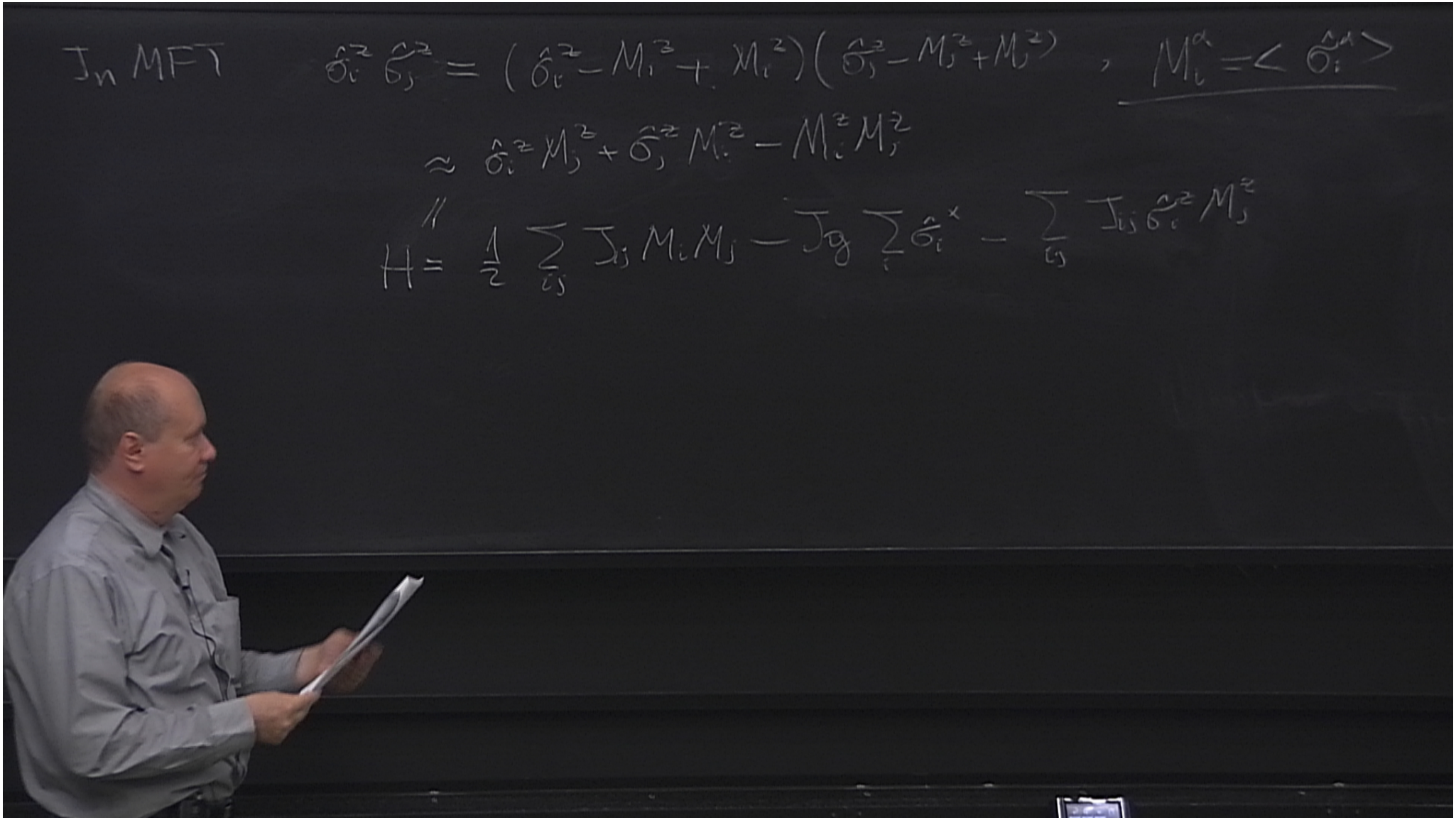
not H for qpt.

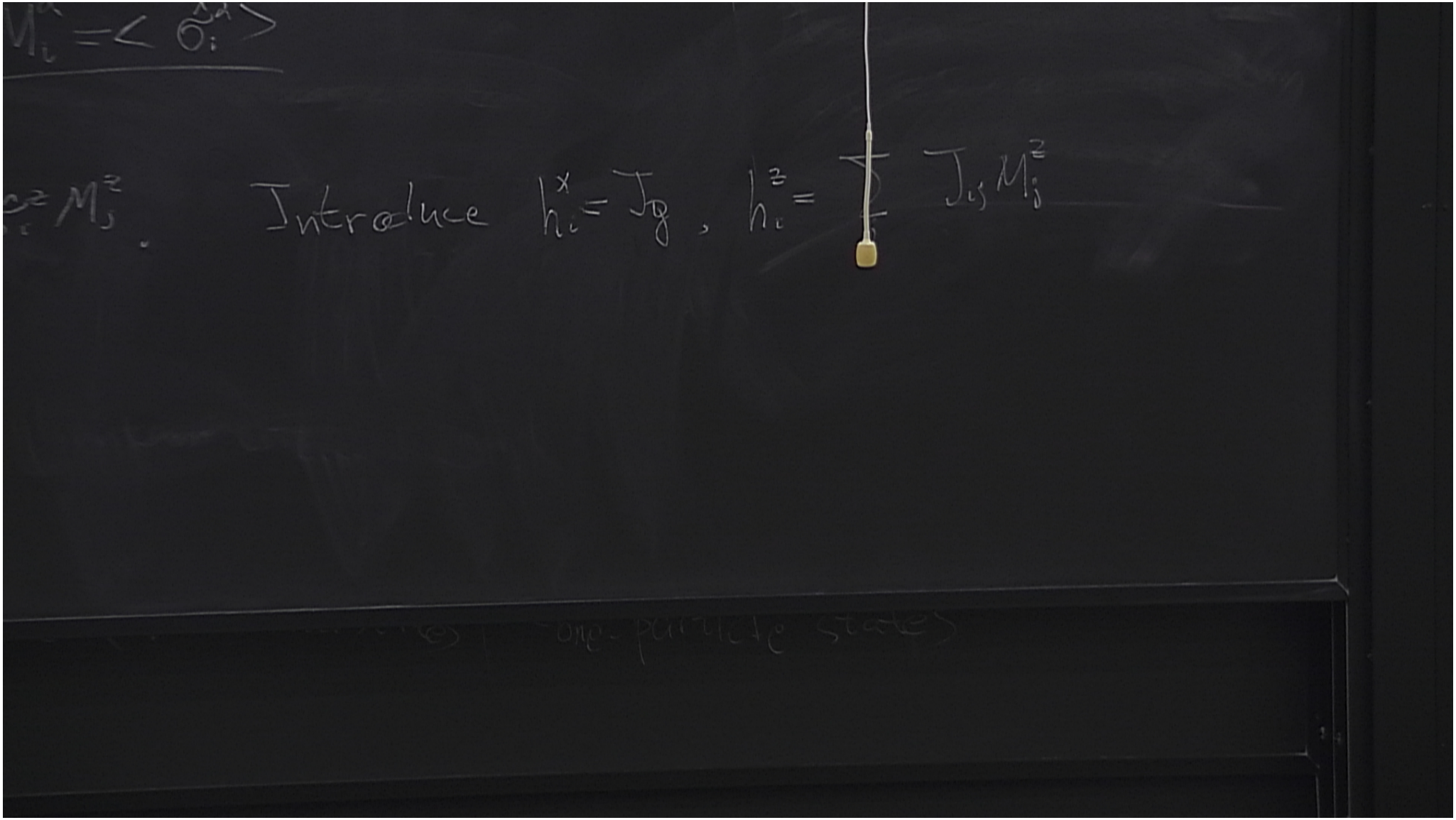

Mean-field theory (MFT)
$H_I = -gJ \sum_i \hat{\sigma}_i^x + \frac{1}{2} \sum_{i,j} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z$
$J_{ij} = J(\vec{r}_i - \vec{r}_j)$
↓sum over all sites $J_{ii} = 0$


Mean-field theory (MFT)
$H_I = -gJ\sum_i \hat{\sigma}_i^x + \frac{1}{2}\sum_{i,j} J_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z$
$J_{ij} = J(\vec{r}_i - \vec{r}_j)$
↓sum over all sites $J_{ii}=0$
$J(\vec{q}) = \sum_{\vec{r}} e^{i\vec{q}\vec{r}} J(\vec{r}) = 2J\sum_{d=1}^{d} \cos q_1 a$
$\Longrightarrow J(\vec{0}) = 2Jd \equiv zJ$
2d-coordinatio
if nearest-neighbour interactions


$E_{gs}+8dJ$
$E_{gs}+4(2d-1)J$
Mean-field theory (MFT)
$H_I=-gJ\sum_i \hat{\sigma}_i^x+\frac{1}{2}\sum_{i,j} J_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z$
$J_{ij}=J(\vec{r}_i-\vec{r}_j)$
↓sum over all sites $J_{ii}=0$
$J(\vec{q})=\sum_{\vec{r}} e^{i\vec{q}\vec{r}}J(\vec{r})=2J\sum_{d=1}^{d}\cos q_d a$
$\Longrightarrow J(\vec{0})=2Jd\equiv\frac{z}{2}J$
2d-coordination number
if nearest-neighbour interactions
a- lattice spacing


$E_{GS} + 8dJ$
$E_{GS} + 4(2d-1)J$
Mean-field theory (MFT)
$H_I = -gJ \sum_i \hat{\sigma}_i^x - \frac{1}{2} \sum_{i,j} J_{ij} \hat{\sigma}_i^z \hat{\sigma}_j^z$
$J_{ij} = J(\vec{r}_i - \vec{r}_j)$
↓ sum over all sites $J_{ii} = 0$
$J(\vec{q}) = \sum_{\vec{r}} e^{i\vec{q}\vec{r}} J(\vec{r}) = 2J \sum_{d=1}^{d} \cos q_d a$
$\Longrightarrow$
$J(\vec{0}) = 2Jd \equiv \frac{z}{2} J$
2d-coordination number
d nearest-neighbour interactions
a- lattice spacing


In MFT
$\hat{\sigma}_i^z \hat{\sigma}_j^z = (\hat{\sigma}_i^z - M_i^z + M_i^z)(\hat{\sigma}_j^z - M_j^z + M_j^z)$, $M_i^\alpha = \langle \hat{\sigma}_i^\alpha \rangle$
$\approx \hat{\sigma}_i^z M_j^z + \hat{\sigma}_j^z M_i^z - M_i^z M_j^z$
$H = \frac{1}{2} \sum_{ij} J_{ij} M_i M_j - J_g \sum_i \hat{\sigma}_i^x - \sum_{ij} J_{ij} \hat{\sigma}_i^z M_j^z$


$M_i^x = \langle \hat{\sigma}_i^x \rangle$
M_j^z
Introduce $h_i^x = J_g$, $h_i^z = \sum_j J_{ij} M_j^z$

$$\hat{\sigma}_i^z \hat{\sigma}_j^z = (\hat{\sigma}_i^z - M_i^z + M_i^z)(\hat{\sigma}_j^z - M_j^z + M_j^z) \quad , \quad \underline{M_i^\alpha = \langle \hat{\sigma}_i^\alpha \rangle}$$

$$\approx \hat{\sigma}_i^z M_j^z + \hat{\sigma}_j^z M_i^z - M_i^z M_j^z$$

$$H = \frac{1}{2} \sum_{ij} J_{ij} M_i^z M_j^z - J_g \sum_i \hat{\sigma}_i^x - \sum_{ij} J_{ij} \hat{\sigma}_i^z M_j^z \quad \text{Introduc}$$

$$= \frac{1}{2} \sum_{ij} J_{ij} M_i^z M_j^z - \sum_i h_i^x \hat{\sigma}_i^x - \sum_i h_i^z \hat{\sigma}_i^z$$

$M_i = \langle \sigma_i \rangle$

$\hat{\sigma}_i^x - \sum_{ij} J_{ij} \hat{\sigma}_i^z M_j^z$. Introduce $h_i^x = J_g$, $h_i^z = \sum_j J_{ij} M_j^z$

$h_i^x \hat{\sigma}_i^x - \sum_i h_i^z \hat{\sigma}_i^z$, Need to know e/values of $h_i^x \hat{\sigma}_i^x + h_i^z \hat{\sigma}_i^z$

need $H_0, H_1 \neq 0$

$H_1 = -J_g \sum_i \hat{\sigma}_i^x - J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z = g H_0 + H_1$, J ... units of energy

$\langle i,j \rangle$ ... nearest neighbours $\hat{\sigma}_i^\alpha$ - Pauli matrices ...

$\hat{\sigma}_i^z \hat{\sigma}_j^z = (\hat{\sigma}_i^z - M_i^z + M_i^z)(\hat{\sigma}_j^z - M_j^z + M_j^z)$, $M_i^\alpha = \langle \hat{\sigma}_i^\alpha \rangle$

$\approx \hat{\sigma}_i^z M_j^z + \hat{\sigma}_j^z M_i^z - M_i^z M_j^z$

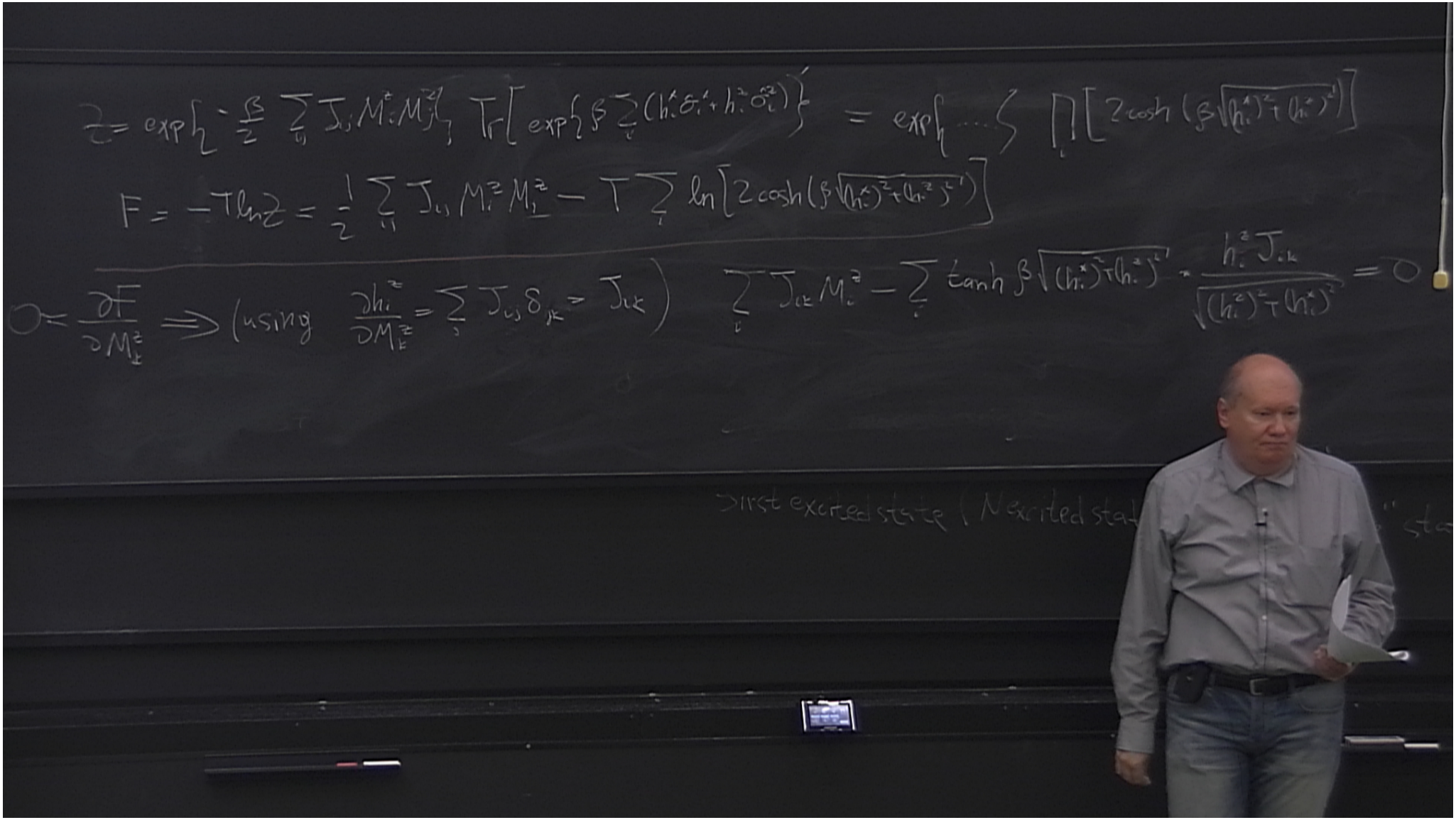
$H = \frac{1}{2} \sum_{ij} J_{ij} M_i^z M_j^z - J_g \sum_i \hat{\sigma}_i^x - \sum_{ij} J_{ij} \hat{\sigma}_i^z M_j^z$. Introduce $h_i^x = J_g$, $h_i^z = \sum_j J_{ij} M_j^z$

$= \frac{1}{2} \sum_{ij} J_{ij} M_i^z M_j^z - \sum_i h_i^x \hat{\sigma}_i^x - \sum_i h_i^z \hat{\sigma}_i^z$, Need to know eValues of $h_i^x \hat{\sigma}_i^x + h_i^z \hat{\sigma}_i^z$

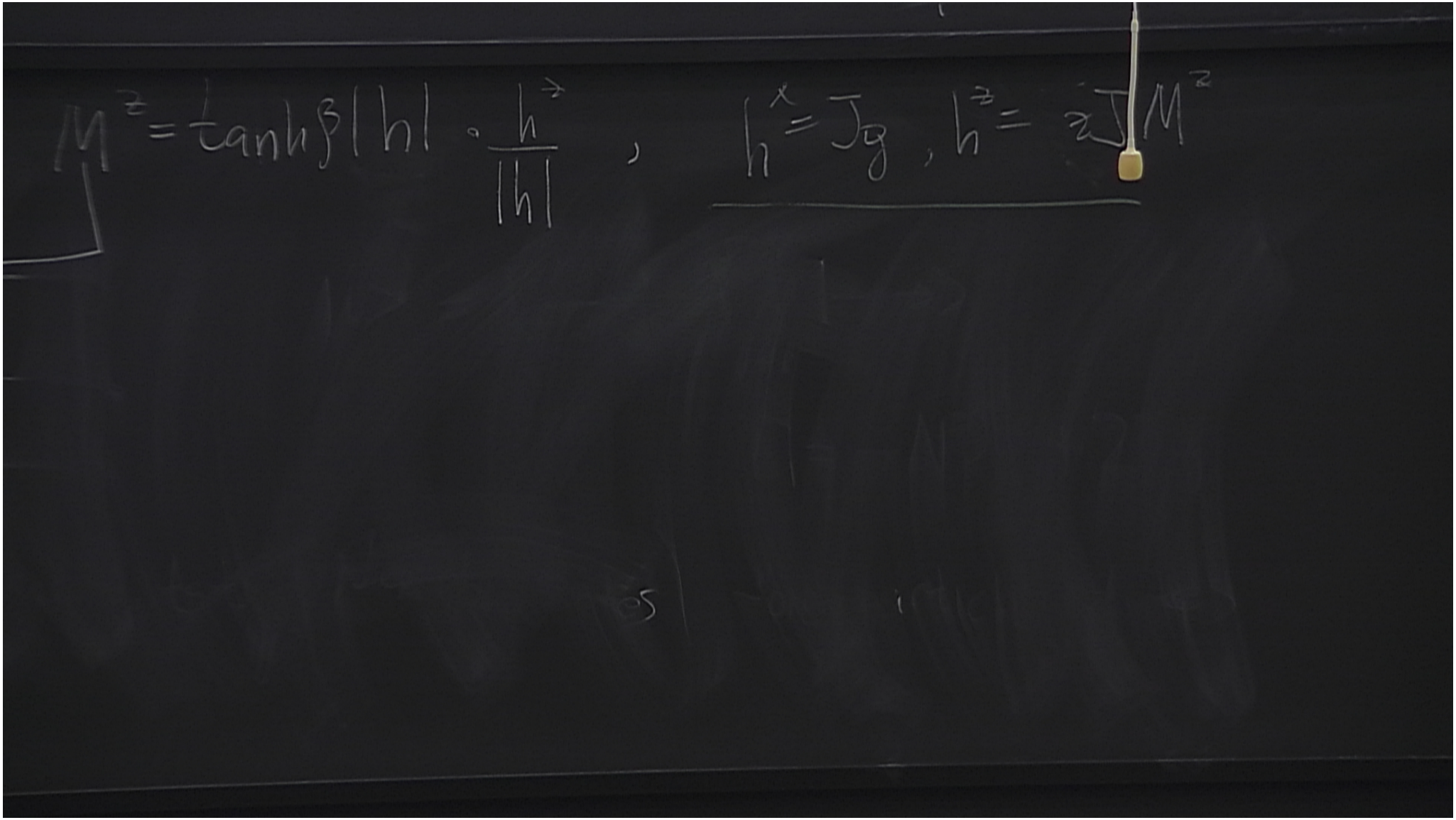
Introduce $h_i^x = J_g$, $h_i^3 = \sum_j J_{ij} M_j$

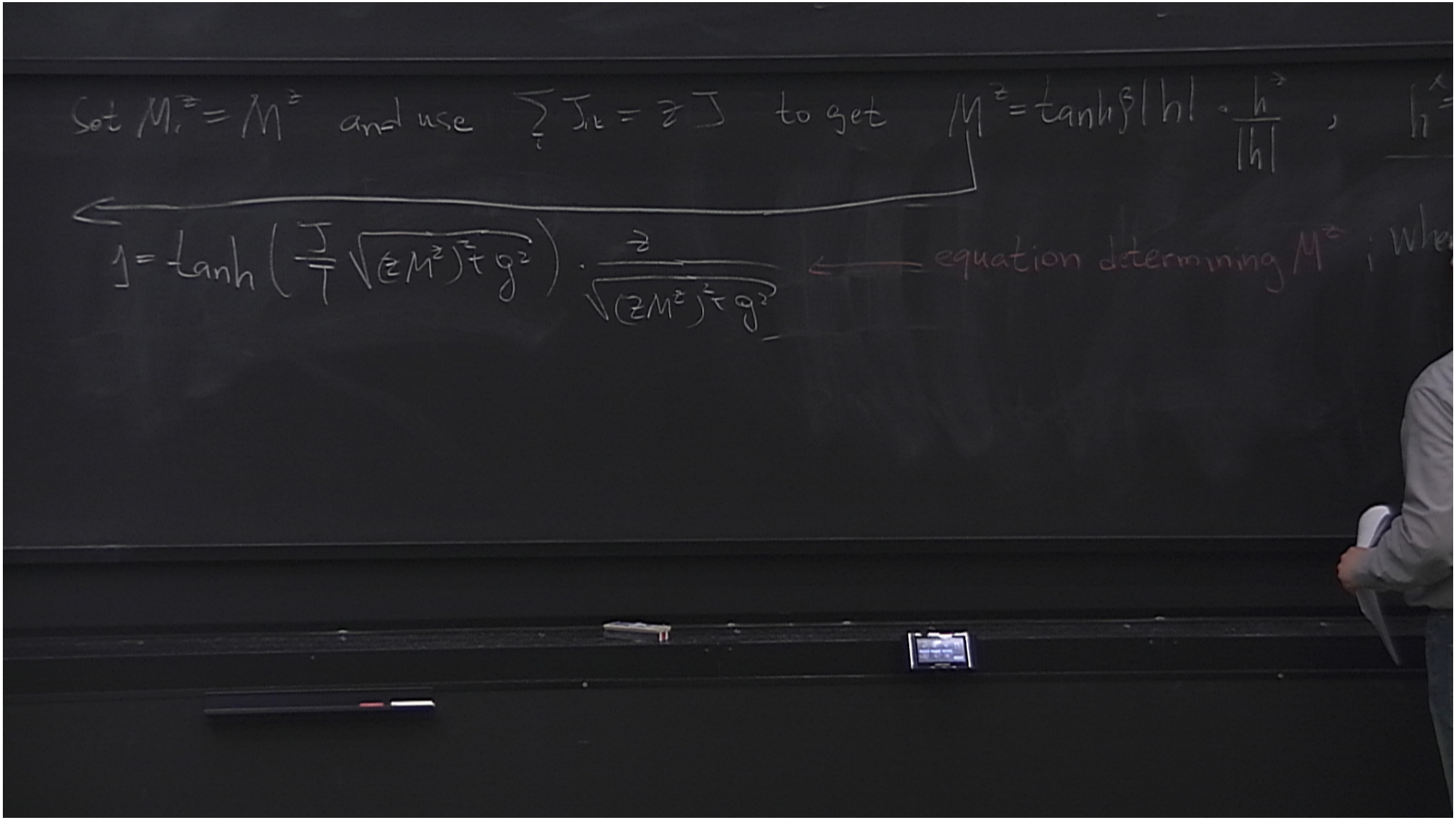
to know e/values of $h_i^x \hat{\sigma}_i^x + h_i^3 \hat{\sigma}_i^z$ that are

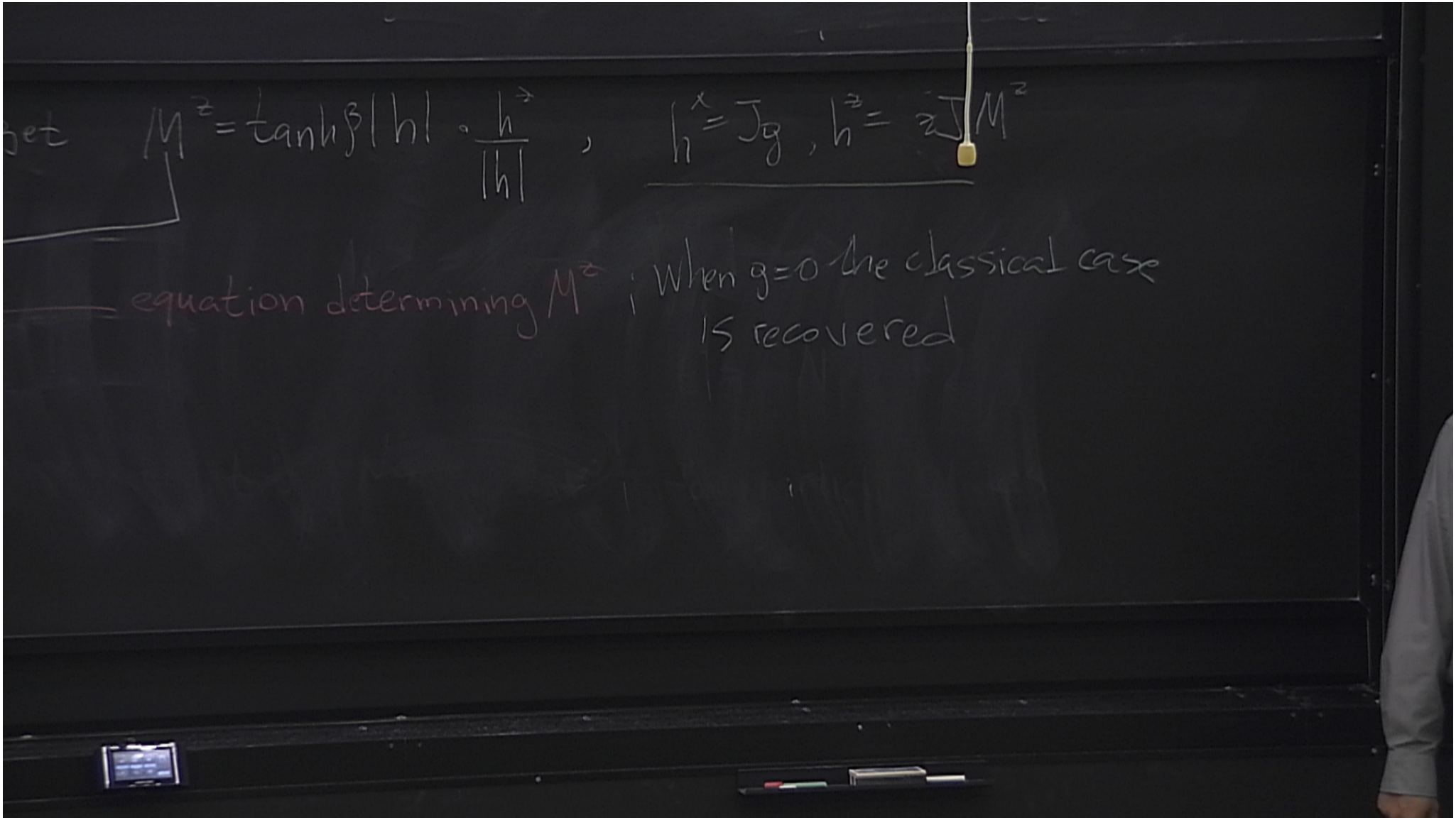
$\pm \sqrt{(h_i^x)^2 + (h_i^3)^2}$

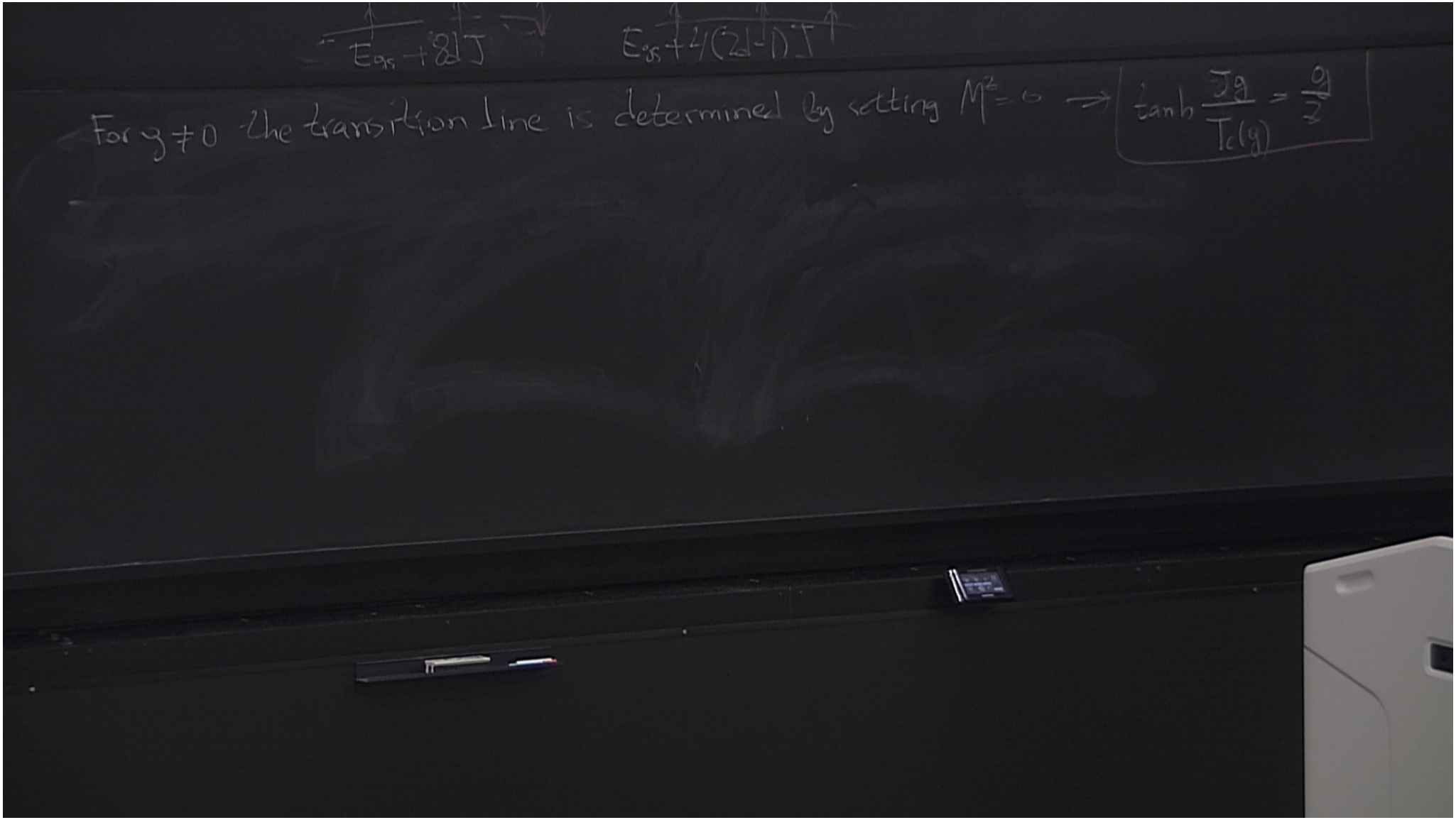

$Z = \exp\{-\frac{\beta}{2}\sum_{ij} J_{ij} M_i^z M_j^z\} \, Tr\left[\exp\{\beta \sum_i (h_i^x \sigma_i^x + h_i^z \sigma_i^z)\}\right] = \exp\{\cdots\} \prod_i \left[2\cosh\left(\beta\sqrt{(h_i^x)^2 + (h_i^z)^2}\right)\right]$
$F = -T \ln Z = \frac{1}{2}\sum_{ij} J_{ij} M_i^z M_j^z - T \sum_i \ln\left[2\cosh\left(\beta\sqrt{(h_i^x)^2 + (h_i^z)^2}\right)\right]$
$0 = \frac{\partial F}{\partial M_k^z} \Rightarrow$ (using $\frac{\partial h_i^z}{\partial M_k^z} = \sum_j J_{ij}\delta_{jk} = J_{ik}$) $\sum_i J_{ik} M_i^z - \sum_i \tanh\beta\sqrt{(h_i^x)^2 + (h_i^z)^2} \cdot \frac{h_i^z J_{ik}}{\sqrt{(h_i^x)^2 + (h_i^z)^2}} = 0$
>irst excited state (Nexcited stat

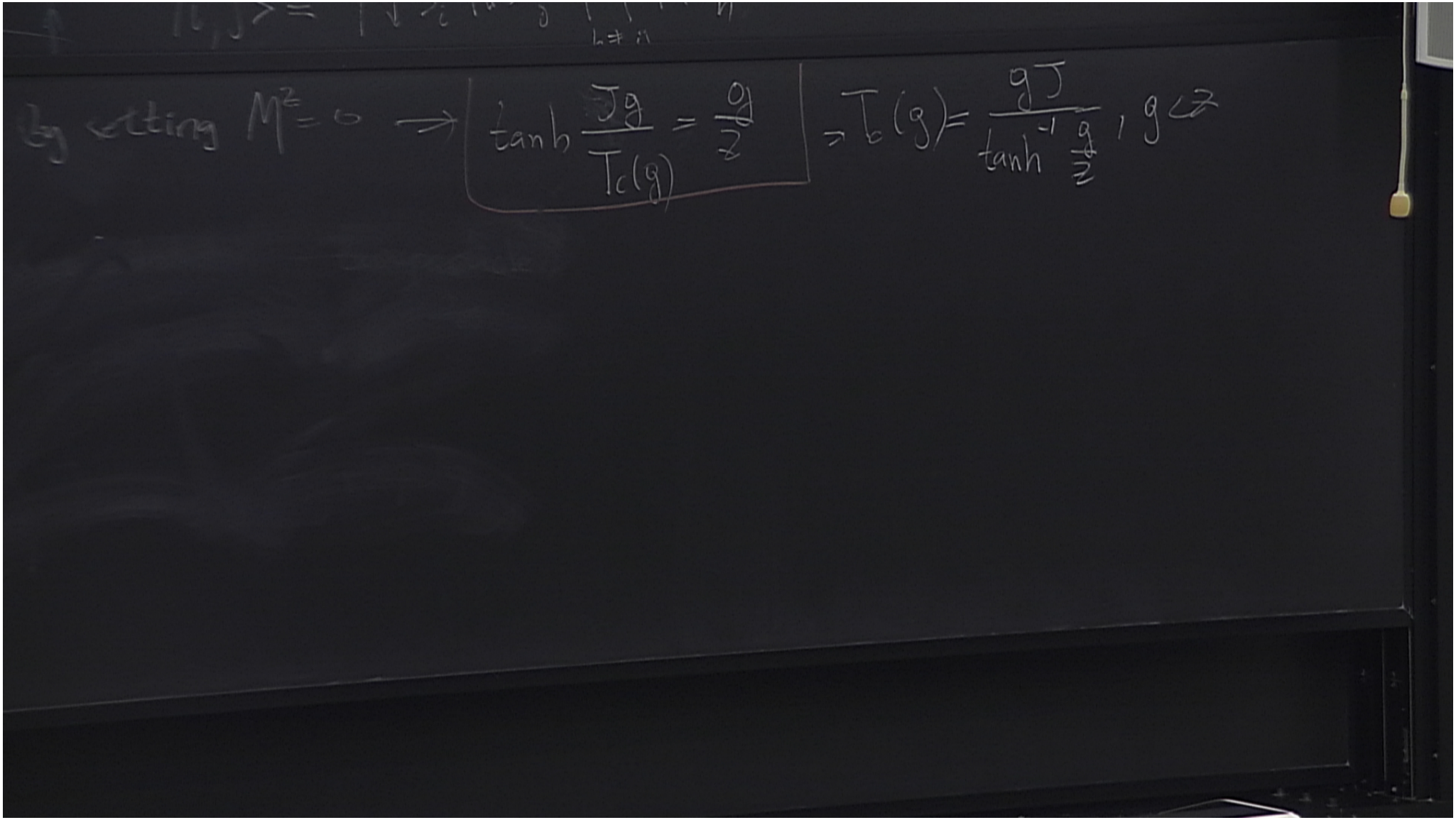
Set $M_i^z = M^z$ and use $\sum_i J_{ik} = zJ$ to get $M^z = \tanh\beta|h| \cdot \frac{\vec{h}}{|h|}$,


$M^z = \tanh\beta|h| \cdot \frac{\vec{h}}{|h|}$,
$h^x = J_g$, $h^z = zJM^z$


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$1 = \tanh\left(\frac{J}{T}\sqrt{(zM^z)^2 + g^2}\right) \cdot \frac{z}{\sqrt{(zM^z)^2 + g^2}}$
equation determining M^z


bet $M^z = \tanh\beta|h| \cdot \frac{\vec{h}}{|h|}$, $h^x = Jg$, $h^z = zJM^z$
equation determining M^z; When $g=0$ the classical case is recovered


$E_{gs} + 8J$
$E_{gs} + 4(2l-1)J$
For $g \neq 0$ the transition line is determined by setting $M^2 = 0 \rightarrow$
$\tanh \frac{Jq}{T_c(q)} = \frac{q}{z}$


by setting $M^2 = 0$ $\rightarrow$ $\tanh \frac{Jg}{T_c(g)} = \frac{g}{z}$ $\Rightarrow T_c(g) = \frac{gJ}{\tanh^{-1} \frac{g}{z}}$; $g <$

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For small g, $T_c(g) = zJ\left(1 - \frac{1}{3}\frac{g^2}{z^2}\right)$

$t_{ac} = -N J a$

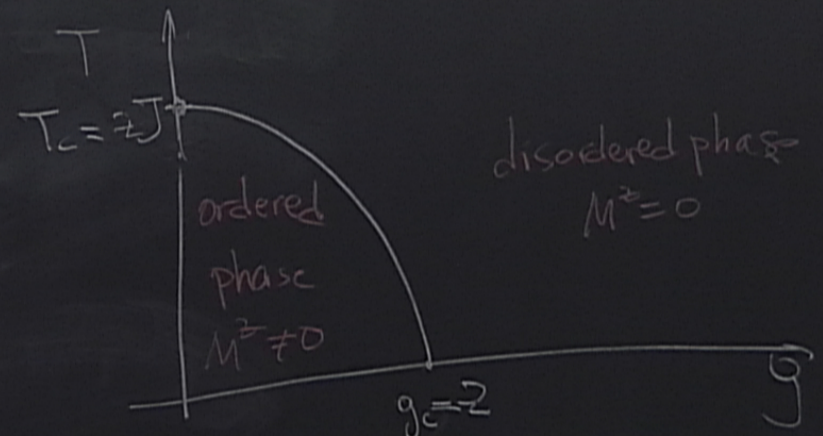
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For small g, $T_c(g) = zJ\left(1 - \frac{1}{3}\frac{g^2}{z^2}\right)$

Setting $T_c(g) = 0$ we get $g_c = z$ — quantum critical point

$\left(\text{For small } T_c(g) - g = z\left(1 - 2\exp\left\{-\frac{zJ}{T_c(g)}\right\}\right)\right)$

el by setting $M^2 = 0$ $\rightarrow$ $\tanh \frac{Jq}{T_c(q)} = \frac{q}{z}$ $\Rightarrow T_c(q) = \frac{qJ}{\tanh^{-1}\frac{q}{z}}$, $q < z$



critical point

$\frac{zJ}{T_c(q)}$

z-coordination number

a- lattice spacing