Title: PSI 2018/2019 - Condensed Matter - Lecture 7

Date: Nov 20, 2018 10:45 AM

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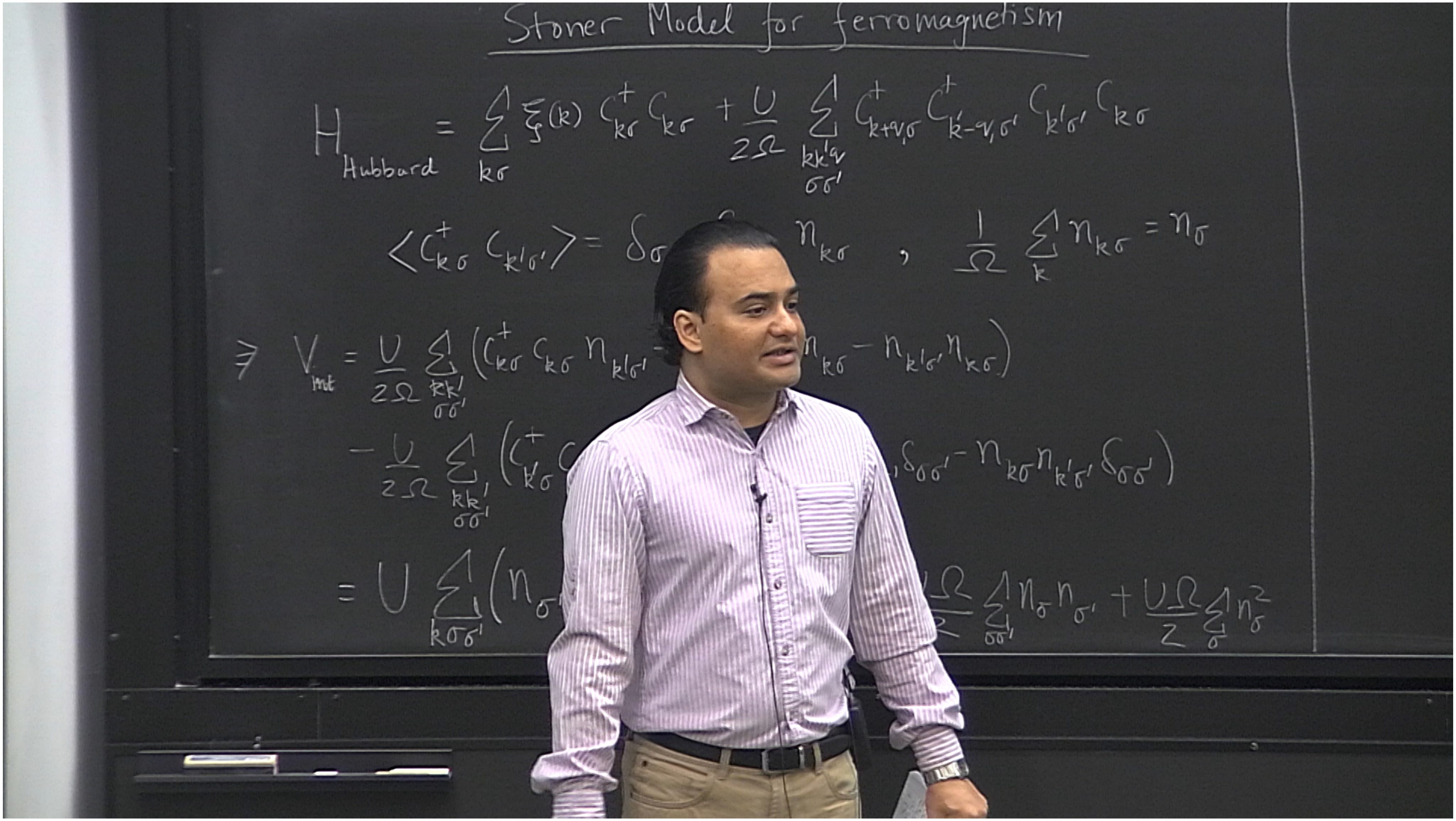
Abstract:


Stoner Model for ferromagnetism
$H_{Hubbard} = \sum_{k\sigma} \xi(k) c^{+}_{k\sigma} c_{k\sigma} + \frac{U}{2\Omega} \sum_{kk'q,\sigma\sigma'} c^{+}_{k+q,\sigma} c^{+}_{k'-q,\sigma'} c_{k'\sigma'} c_{k\sigma}$
$\frac{1}{\Omega} \sum_{k} n_{k\sigma} = n_\sigma$

Stoner Model for ferromagnetism

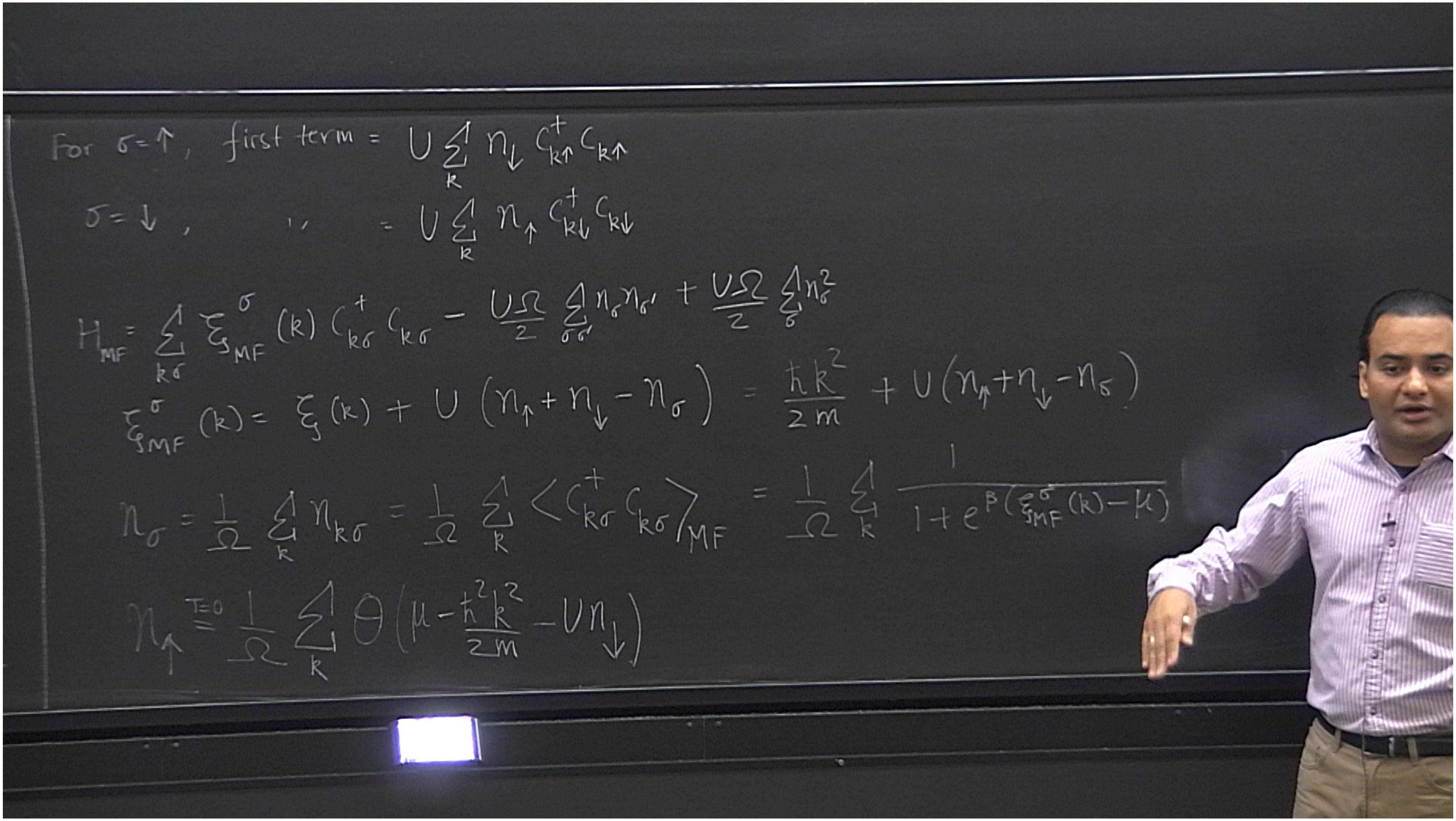
$$H_{\text{Hubbard}} = \sum_{k\sigma} \xi(k)\, c^{\dagger}_{k\sigma} c_{k\sigma} + \frac{U}{2\Omega} \sum_{\substack{kk'q \\ \sigma\sigma'}} c^{\dagger}_{k+q,\sigma}\, c^{\dagger}_{k'-q,\sigma'}\, c_{k'\sigma'}\, c_{k\sigma}$$

$$\langle c^{\dagger}_{k\sigma}\, c_{k'\sigma'} \rangle = \delta_{\sigma\sigma'}\, \delta_{kk'}\, n_{k\sigma} \quad , \quad \frac{1}{\Omega} \sum_{k} n_{k\sigma} = n_{\sigma}$$

$$\Rightarrow V_{\text{int}} = \frac{U}{2\Omega} \sum_{\substack{kk' \\ \sigma\sigma'}} \left(c^{\dagger}_{k\sigma} c_{k\sigma}\, n_{k'\sigma'} + c^{\dagger}_{k'\sigma'} c_{k'\sigma'}\, n_{k\sigma} - n_{k'\sigma'} n_{k\sigma} \right)$$

$$- \frac{U}{2\Omega} \sum_{\substack{kk' \\ \sigma\sigma'}} \left(c^{\dagger}_{k'\sigma} c_{k'\sigma'}\, n_{k\sigma} + c^{\dagger}_{k\sigma'} c_{k\sigma}\, n_{k'\sigma'} \delta_{\sigma\sigma'} - n_{k\sigma} n_{k'\sigma'} \delta_{\sigma\sigma'} \right)$$

$$= U \sum_{k\sigma\sigma'} \left(n_{\sigma'} - n_{\sigma} \delta_{\sigma\sigma'} \right) c^{\dagger}_{k\sigma} c_{k\sigma} - \frac{U\Omega}{2} \sum_{\sigma\sigma'} n_{\sigma} n_{\sigma'} + \frac{U\Omega}{2} \sum_{\sigma} n_{\sigma}^{2}$$



For $\sigma=\uparrow$, first term $= U\sum_k n_\downarrow c^\dagger_{k\uparrow} c_{k\uparrow}$
$\sigma=\downarrow$, '' $= U\sum_k n_\uparrow c^\dagger_{k\downarrow} c_{k\downarrow}$
$H_{MF} = \sum_{k\sigma} \xi^\sigma_{MF}(k)\, c^\dagger_{k\sigma} c_{k\sigma} - \frac{U\Omega}{2}\sum_{\sigma\sigma'} n_\sigma n_{\sigma'} + \frac{U\Omega}{2}\sum_\sigma n_\sigma^2$
$\xi^\sigma_{MF}(k) = \xi(k) + U(n_\uparrow + n_\downarrow - n_\sigma) = \frac{\hbar k^2}{2m} + U(n_\uparrow + n_\downarrow - n_\sigma)$
$n_\sigma = \frac{1}{\Omega}\sum_k n_{k\sigma} = \frac{1}{\Omega}\sum_k \langle c^\dagger_{k\sigma} c_{k\sigma}\rangle_{MF} = \frac{1}{\Omega}\sum_k \frac{1}{1+e^{\beta(\xi^\sigma_{MF}(k)-\mu)}}$
$n_\uparrow \overset{T=0}{=} \frac{1}{\Omega}\sum_k \Theta\left(\mu - \frac{\hbar^2 k^2}{2m} - U n_\downarrow\right)$

11) Fermionic rules
12) Yukawa diags
13) Atz Maxwell
14) $A^M = 4\times 4$

GR | SAM

a   1-a

For $\sigma=\uparrow$, first term $= U\sum_k n_\downarrow c^\dagger_{k\uparrow} c_{k\uparrow}$

$\sigma=\downarrow$, " $= U\sum_k n_\uparrow c^\dagger_{k\downarrow} c_{k\downarrow}$

$$H_{MF} = \sum_{k\sigma} \xi^\sigma_{MF}(k)\, c^\dagger_{k\sigma} c_{k\sigma} - \frac{U\Omega}{2}\sum_{\sigma\sigma'} n_\sigma n_{\sigma'} + \frac{U\Omega}{2}\sum_\sigma n_\sigma^2$$

$$\xi^\sigma_{MF}(k) = \xi(k) + U(n_\uparrow + n_\downarrow - n_\sigma) = \frac{\hbar k^2}{2m} + U(n_\uparrow + n_\downarrow - n_\sigma)$$

$$n_\sigma = \frac{1}{\Omega}\sum_k n_{k\sigma} = \frac{1}{\Omega}\sum_k \langle c^\dagger_{k\sigma} c_{k\sigma}\rangle_{MF} = \frac{1}{\Omega}\sum_k \frac{1}{1+e^{\beta(\xi^\sigma_{MF}(k)-\mu)}}$$

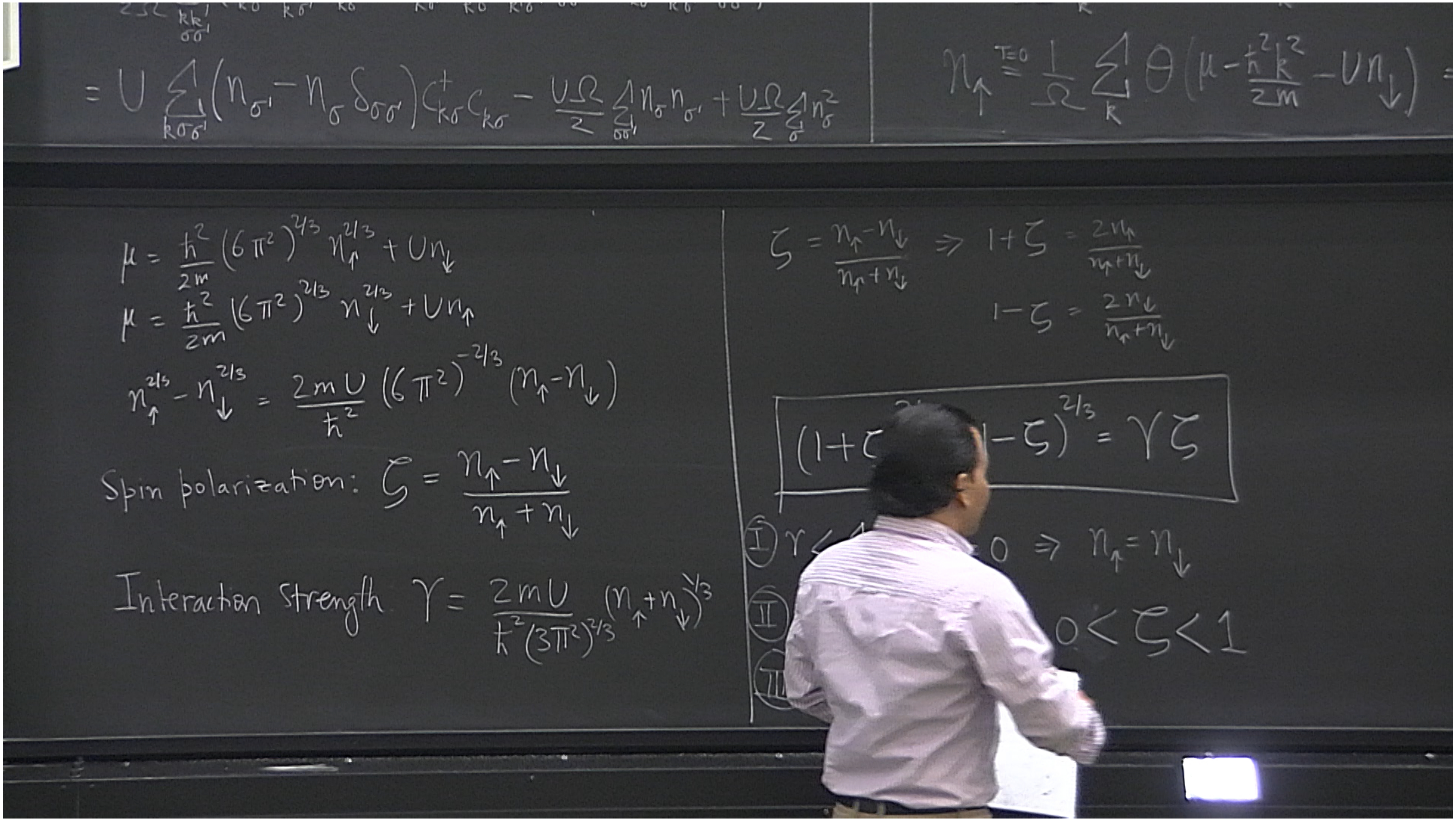
$$n_\uparrow \overset{T=0}{=} \frac{1}{\Omega}\sum_k \Theta\left(\mu - \frac{\hbar^2 k^2}{2m} - Un_\downarrow\right) = \int \frac{d^3k}{(2\pi)^3}\Theta\left(\mu - \frac{\hbar^2k^2}{2m} - Un_\downarrow\right) = \int_0^{k_{F\uparrow}} \frac{dk}{2\pi^2} k^2 = \frac{k_{F\uparrow}^3}{6\pi^2} \quad \& \quad \mu - \frac{\hbar^2 k_{F\uparrow}^2}{2m} - Un_\downarrow = 0$$

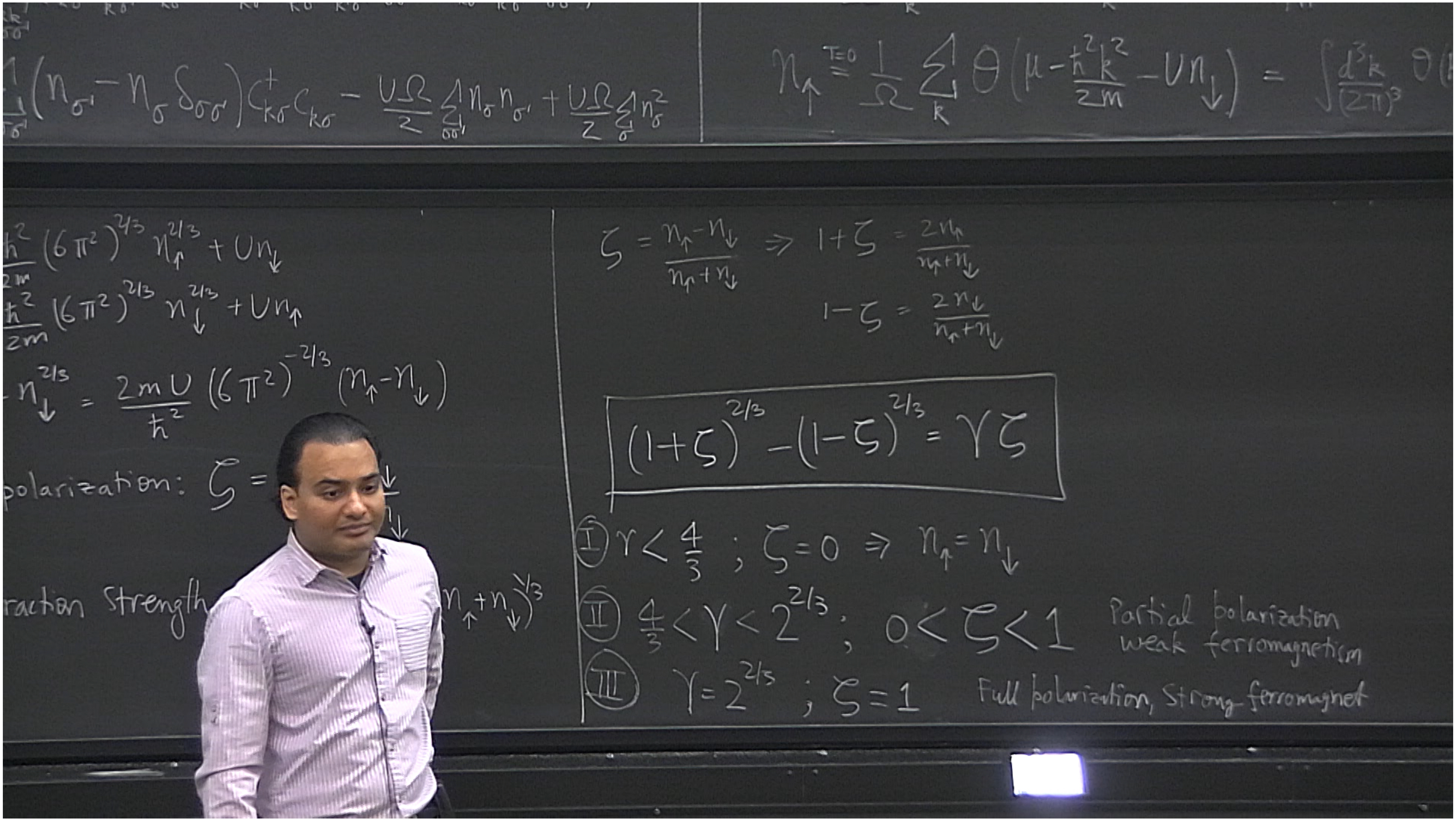
$$n_\downarrow = \frac{k_{F\downarrow}^3}{6\pi^2}$$

$$\mu - \frac{\hbar^2 k_{F\downarrow}^2}{2m} - Un_\uparrow = 0$$

$$\mu = \frac{\hbar^2 k_{F\uparrow}^2}{2m} + Un_\downarrow \qquad \& \qquad k_{F\uparrow} = (6\pi^2 n_\uparrow)^{1/3}$$

$$\mu = \frac{\hbar^2 k_{F\downarrow}^2}{2m} + Un_\uparrow \qquad\qquad k_{F\downarrow} = (6\pi^2 n_\downarrow)^{1/3}$$


$= U \sum_{k\sigma\sigma'} (n_{\sigma'} - n_\sigma \delta_{\sigma\sigma'}) c^\dagger_{k\sigma} c_{k\sigma} - \frac{U\Omega}{2} \sum_{\sigma\sigma'} n_\sigma n_{\sigma'} + \frac{U\Omega}{2} \sum_\sigma n_\sigma^2$
$n_\uparrow \overset{T=0}{=} \frac{1}{\Omega} \sum_k \theta\left(\mu - \frac{\hbar^2 k^2}{2m} - U n_\downarrow\right)$
$\mu = \frac{\hbar^2}{2m} (6\pi^2)^{2/3} n_\uparrow^{2/3} + U n_\downarrow$
$\mu = \frac{\hbar^2}{2m} (6\pi^2)^{2/3} n_\downarrow^{2/3} + U n_\uparrow$
$n_\uparrow^{2/3} - n_\downarrow^{2/3} = \frac{2mU}{\hbar^2} (6\pi^2)^{-2/3} (n_\uparrow - n_\downarrow)$
Spin polarization: $\zeta = \frac{n_\uparrow - n_\downarrow}{n_\uparrow + n_\downarrow}$
Interaction strength $\gamma = \frac{2mU}{\hbar^2 (3\pi^2)^{2/3}} (n_\uparrow + n_\downarrow)^{1/3}$
$\zeta = \frac{n_\uparrow - n_\downarrow}{n_\uparrow + n_\downarrow} \Rightarrow 1 + \zeta = \frac{2n_\uparrow}{n_\uparrow + n_\downarrow}$
$1 - \zeta = \frac{2n_\downarrow}{n_\uparrow + n_\downarrow}$
$(1+\zeta \;\; -\zeta)^{2/3} = \gamma\zeta$
I $\gamma <$ $0 \Rightarrow n_\uparrow = n_\downarrow$
II $0 < \zeta < 1$
III



$\zeta = \frac{n_\uparrow - n_\downarrow}{n_\uparrow + n_\downarrow} \Rightarrow 1+\zeta = \frac{2n_\uparrow}{n_\uparrow + n_\downarrow}$
$1-\zeta = \frac{2n_\downarrow}{n_\uparrow + n_\downarrow}$
$(1+\zeta)^{2/3} - (1-\zeta)^{2/3} = \gamma\zeta$
I $\gamma < \frac{4}{3}$; $\zeta = 0 \Rightarrow n_\uparrow = n_\downarrow$
II $\frac{4}{3} < \gamma < 2^{2/3}$; $0 < \zeta < 1$
Partial polarization
weak ferromagnetism
III $\gamma = 2^{2/3}$; $\zeta = 1$
Full polarization, Strong ferromagnet
polarization: $\zeta =$
raction Strength

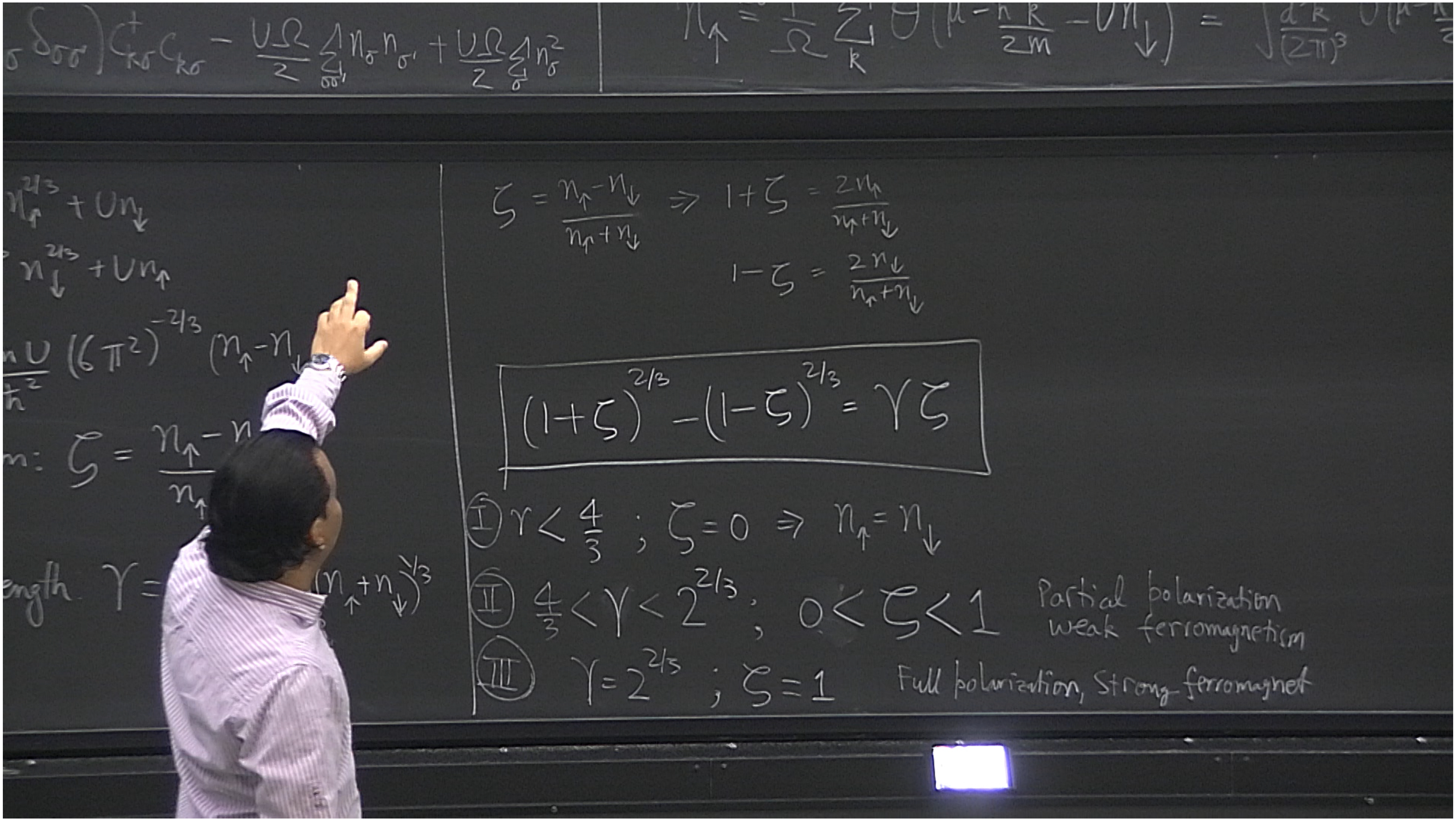
$$\mu = \frac{\hbar^2}{2m}(6\pi^2)^{2/3} n_\uparrow^{2/3} + U n_\downarrow$$

$$\mu = \frac{\hbar^2}{2m}(6\pi^2)^{2/3} n_\downarrow^{2/3} + U n_\uparrow$$

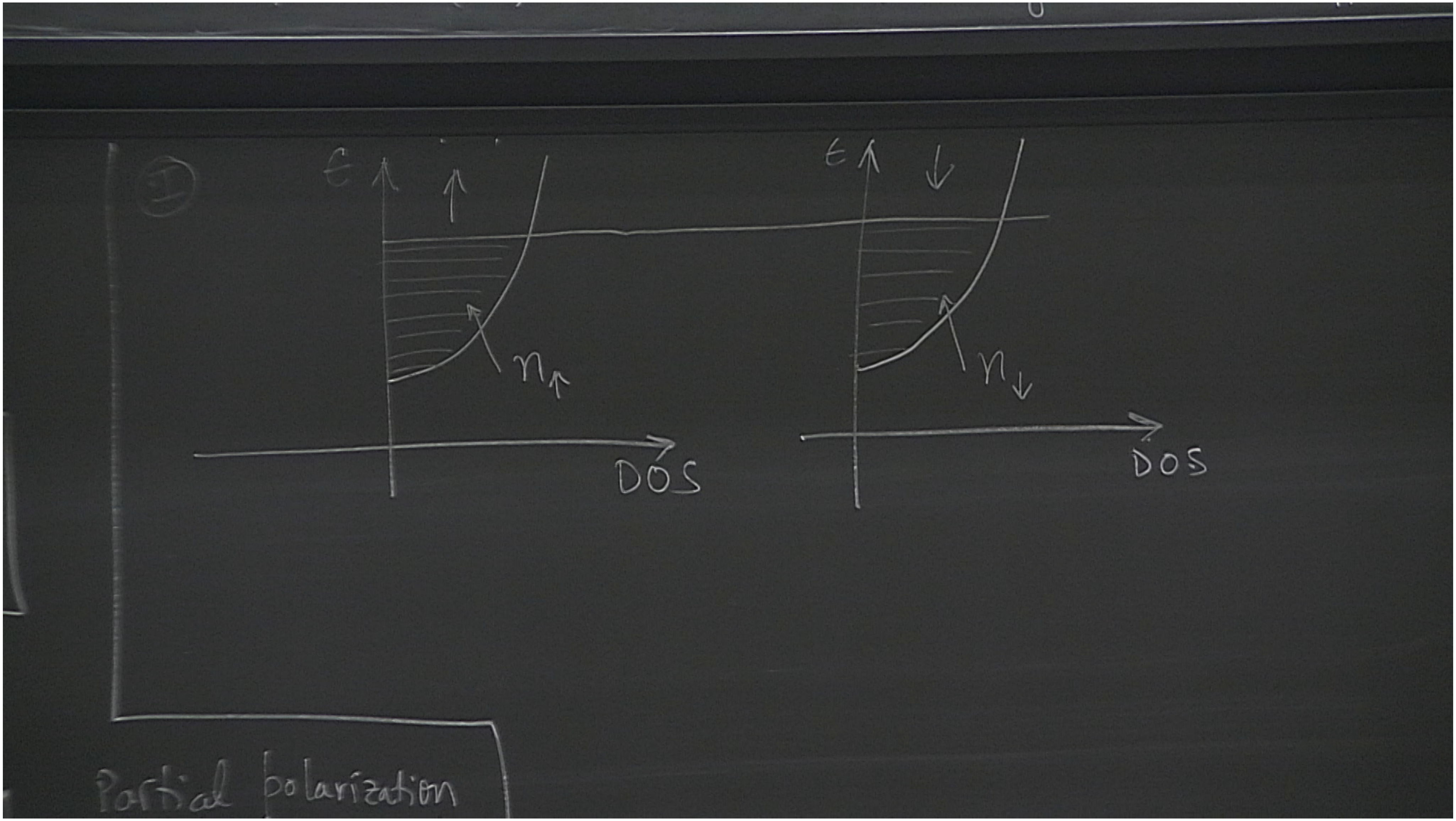
$$n_\uparrow^{2/3} - n_\downarrow^{2/3} = \frac{2mU}{\hbar^2}(6\pi^2)^{-2/3}(n_\uparrow - n_\downarrow)$$

Spin polarization: $\zeta = \dfrac{n_\uparrow - n_\downarrow}{n_\uparrow + n_\downarrow}$

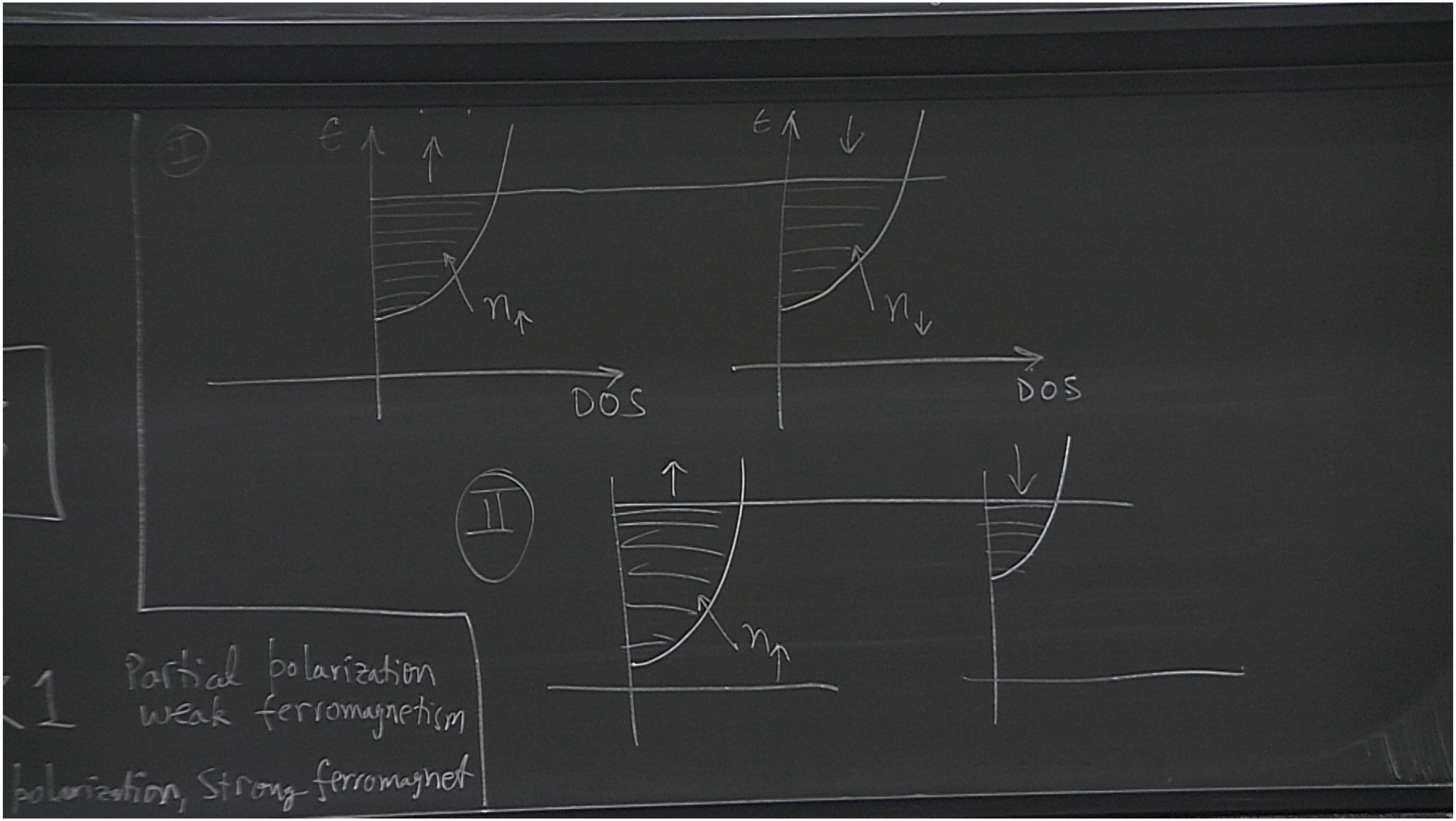
Interaction strength: $\gamma = \dfrac{2mU}{\hbar^2 (3\pi^2)^{2/3}}(n_\uparrow + n_\downarrow)^{1/3}$

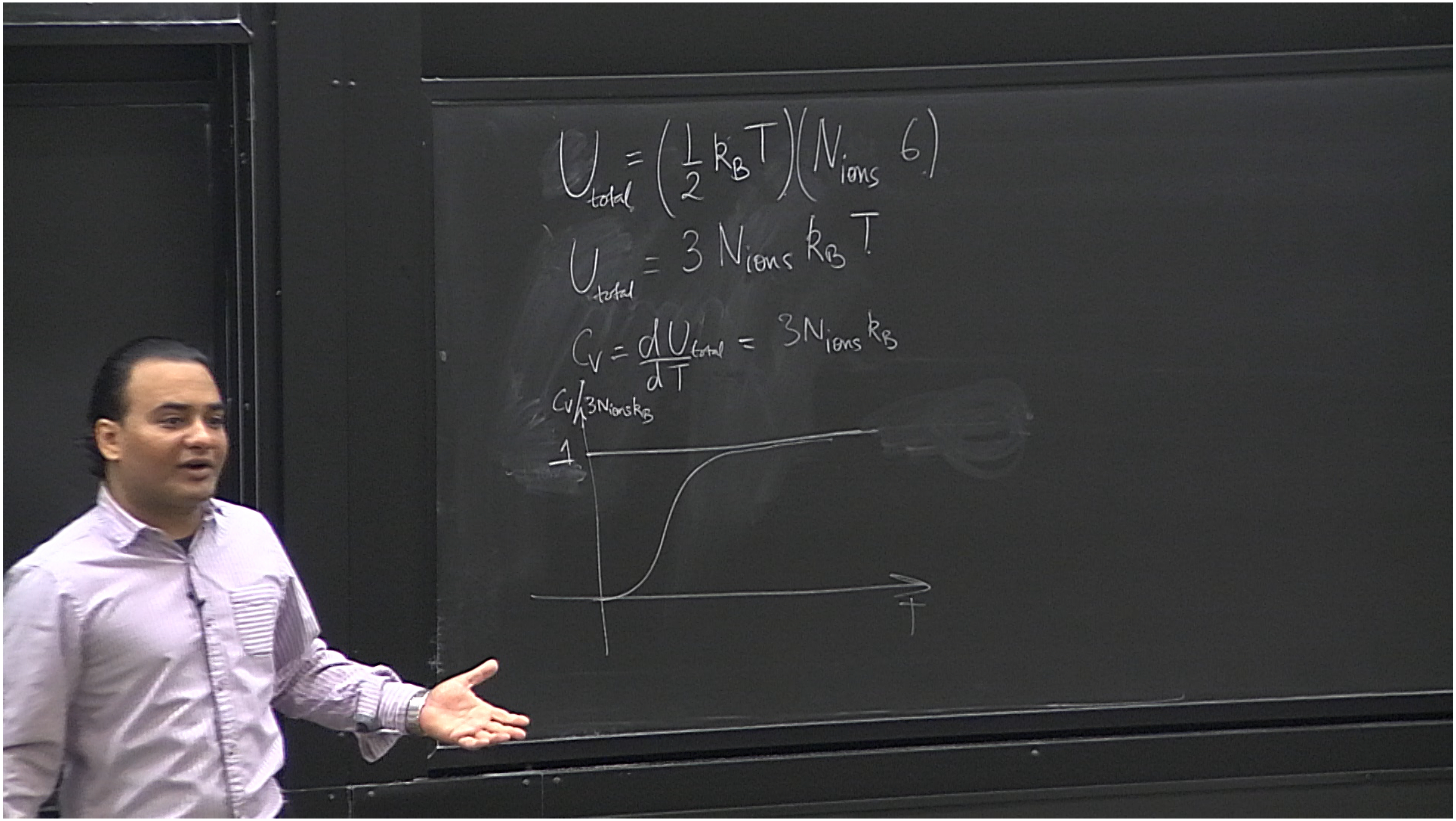


$\zeta = \frac{n_\uparrow - n_\downarrow}{n_\uparrow + n_\downarrow} \Rightarrow 1+\zeta = \frac{2n_\uparrow}{n_\uparrow + n_\downarrow}$
$1-\zeta = \frac{2n_\downarrow}{n_\uparrow + n_\downarrow}$
$(1+\zeta)^{2/3} - (1-\zeta)^{2/3} = \gamma\zeta$
I $\gamma < \frac{4}{3}$; $\zeta = 0 \Rightarrow n_\uparrow = n_\downarrow$
II $\frac{4}{3} < \gamma < 2^{2/3}$; $0 < \zeta < 1$
Partial polarization
weak ferromagnetism
III $\gamma = 2^{2/3}$; $\zeta = 1$
Full polarization, Strong ferromagnet



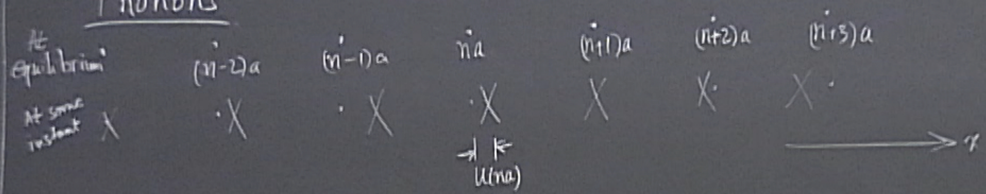
I
ε
↑
$n_\uparrow$
DOS
ε
↓
$n_\downarrow$
DOS
Partial polarization


I
ε
↑
$n_\uparrow$
DOS
ε
↓
$n_\downarrow$
DOS
II
↑
$n_\uparrow$
↓
Partial polarization
weak ferromagnetism
polarization, Strong ferromagnet



$U_{total} = \left(\frac{1}{2} k_B T\right)\left(N_{ions}\ 6\right)$
$U_{total} = 3 N_{ions} k_B T$
$C_V = \frac{dU_{total}}{dT} = 3 N_{ions} k_B$
$C_V / 3 N_{ions} k_B$
1
T

Phonons



$$U = \frac{1}{2}\sum_{\substack{i \\ j\neq i}} V(|\bar{r}_i - \bar{r}_j|) = \frac{1}{2}\sum_{i,j\neq i} V(|\bar{R}_{ij} + \bar{u}_{ij}|) = \frac{1}{2}\sum_{i,j\neq i} V(|\bar{R}_i - \bar{R}_j|) + \cancel{\frac{1}{2}\sum_{i,j\neq i} \frac{\partial V}{\partial x}\Big|_{\bar{R}_{ij}}} \bar{u}_{ij}\cdot\hat{x} + \frac{1}{4}\frac{\partial^2 V}{\partial x^2}\Big|_{\bar{R}_{ij}} (\bar{u}_{ij}\cdot\hat{x})^2 + \ldots$$

$$\bar{r}_i = \bar{R}_i + \bar{u}_i$$
$$\bar{r}_j = \bar{R}_j + \bar{u}_j$$

$$K_{ij} = \frac{\partial^2 V}{\partial x^2}\Big|_{\bar{R}_{ij}}$$

$$U_{nn}^{harm} = \frac{K}{4} \sum_n \left[\left(u(na) - u((n+1)a) \right)^2 + \left(u(na) - u((n-1)a) \right)^2 \right]$$

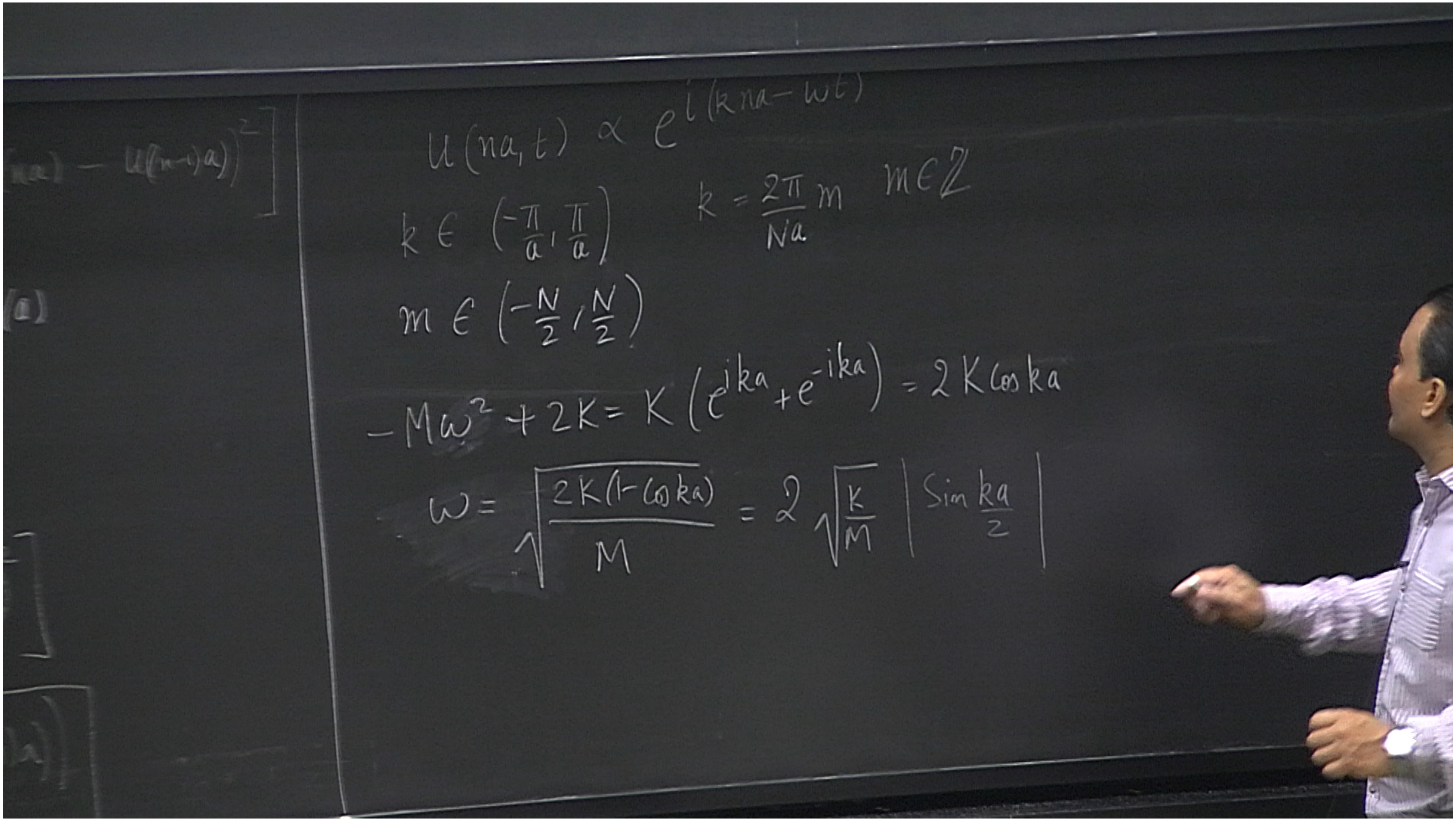
$$u((N+1)a) = u(a)$$

$$K_{ij} = \left. \frac{\partial^2 V}{\partial x^2} \right|_{\bar{R}_{ij}} = K$$

$$\Rightarrow U_{nn}^{harm} = \frac{K}{2} \sum_n \left(u(na) - u((n+1)a) \right)^2$$

$$\mathcal{L} = \sum_n \left[\frac{M}{2} \dot{u}(na)^2 - \frac{K}{2} \left(u(na) - u((n+1)a) \right)^2 \right]$$

$$\boxed{M \ddot{u}(na) = -K \left(2u(na) - u((n+1)a) - u((n-1)a) \right)}$$


$u(na,t) \propto e^{i(kna-\omega t)}$
$k \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right)$
$k = \frac{2\pi}{Na} m \quad m \in \mathbb{Z}$
$m \in \left(-\frac{N}{2}, \frac{N}{2}\right)$
$-M\omega^2 + 2K = K\left(e^{ika} + e^{-ika}\right) = 2K\cos ka$
$\omega = \sqrt{\frac{2K(1-\cos ka)}{M}} = 2\sqrt{\frac{K}{M}}\left|\sin\frac{ka}{2}\right|$

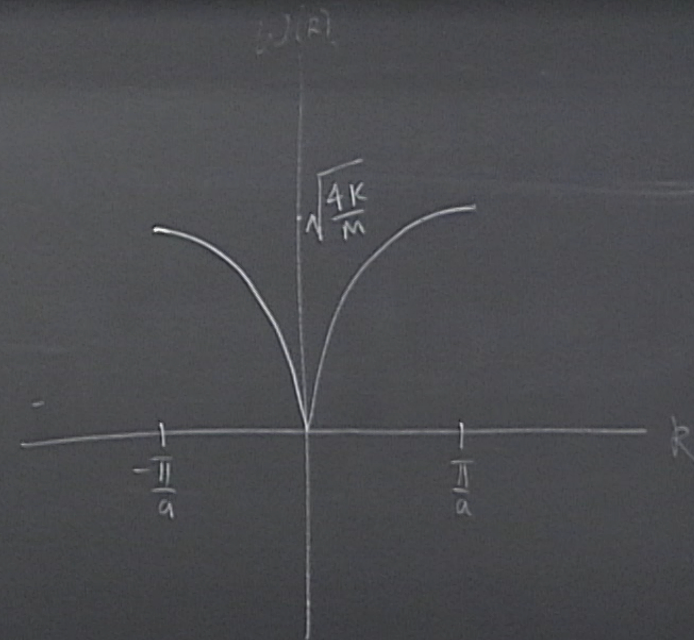
$$u(na,t) \propto e^{i(kna-\omega t)}$$

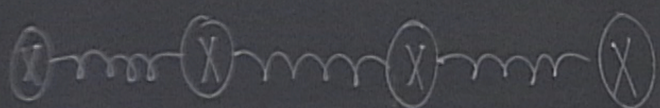
$$k \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right) \qquad k = \frac{2\pi}{Na} m \qquad m \in \mathbb{Z}$$

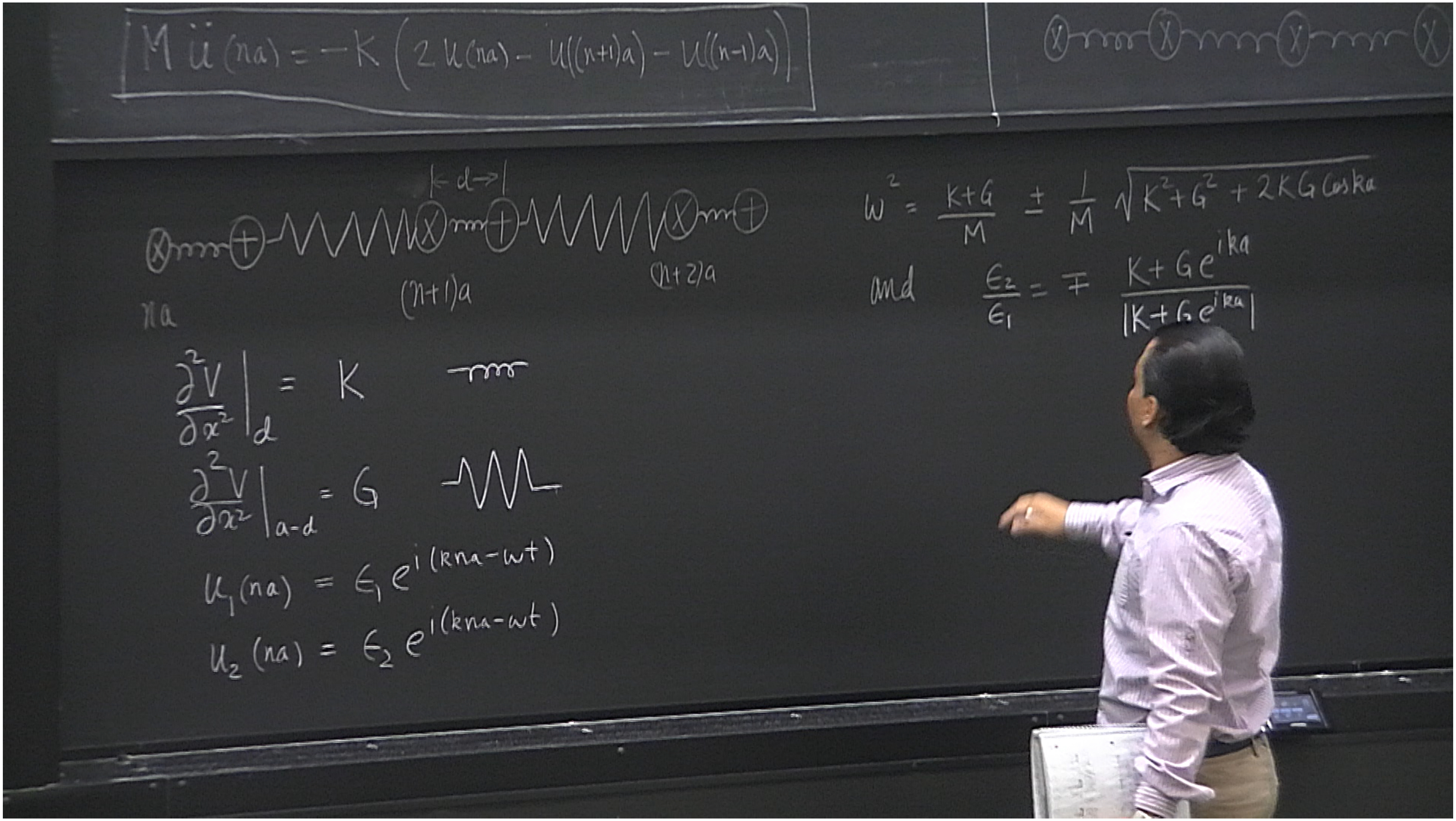
$$m \in \left(-\frac{N}{2}, \frac{N}{2}\right)$$

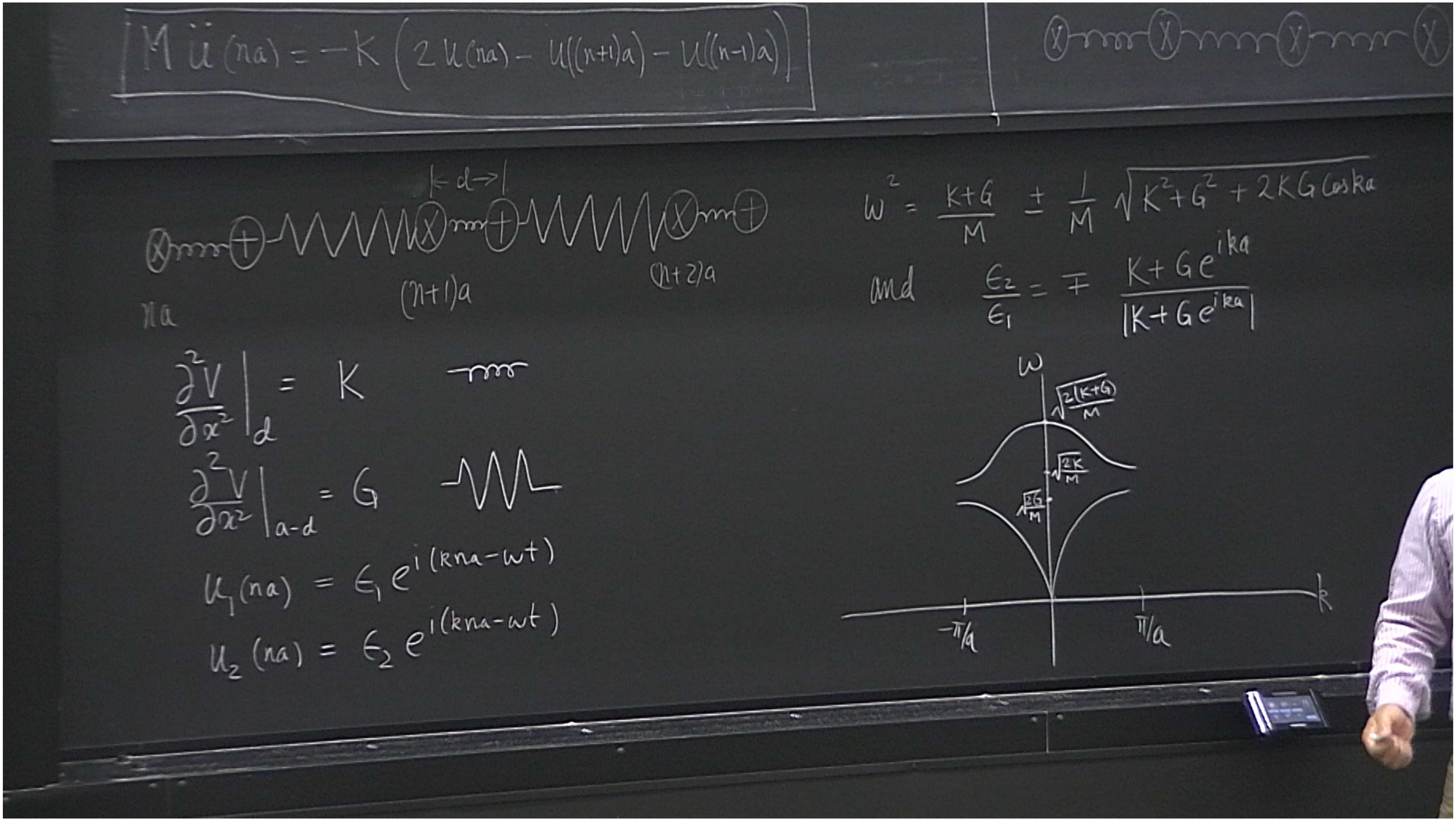
$$-M\omega^2 + 2K = K\left(e^{ika} + e^{-ika}\right) = 2K\cos ka$$

$$\omega = \sqrt{\frac{2K(1-\cos ka)}{M}} = 2\sqrt{\frac{K}{M}}\left|\sin\frac{ka}{2}\right|$$

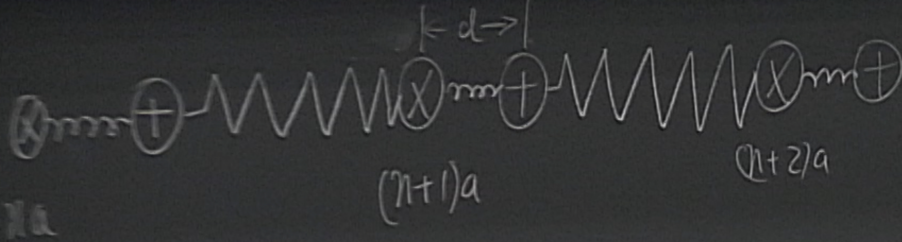





M ü(na) = −K (2 u(na) − u((n+1)a) − u((n−1)a))
|← d →|
na
(n+1)a
(n+2)a
∂²V/∂x² |_d = K
∂²V/∂x² |_(a−d) = G
u₁(na) = ϵ₁ e^(i(kna−ωt))
u₂(na) = ϵ₂ e^(i(kna−ωt))
ω² = (K+G)/M ± (1/M) √(K² + G² + 2KG cos ka)
and ϵ₂/ϵ₁ = ∓ (K + G e^(ika)) / |K + G e^(ika)|


$M\ddot{u}(na) = -K\left(2u(na) - u((n+1)a) - u((n-1)a)\right)$
$\vert\leftarrow d \rightarrow\vert$
na
$(n+1)a$
$(n+2)a$
$\left.\frac{\partial^2 V}{\partial x^2}\right|_d = K$
$\left.\frac{\partial^2 V}{\partial x^2}\right|_{a-d} = G$
$u_1(na) = \epsilon_1 e^{i(kna-\omega t)}$
$u_2(na) = \epsilon_2 e^{i(kna-\omega t)}$
$\omega^2 = \frac{K+G}{M} \pm \frac{1}{M}\sqrt{K^2+G^2+2KG\cos ka}$
and $\frac{\epsilon_2}{\epsilon_1} = \mp \frac{K+Ge^{ika}}{|K+Ge^{ika}|}$
ω
$\sqrt{\frac{2(K+G)}{M}}$
$\sqrt{\frac{2K}{M}}$
$\sqrt{\frac{2G}{M}}$
$-\pi/a$
π/a
k

$$M\ddot{u}(na) = -K\Big(2u(na) - u\big((n+1)a\big) - u\big((n-1)a\big)\Big)$$



$$\left.\frac{\partial^2 V}{\partial x^2}\right|_{d} = K$$

$$\left.\frac{\partial^2 V}{\partial x^2}\right|_{a-d} = G$$

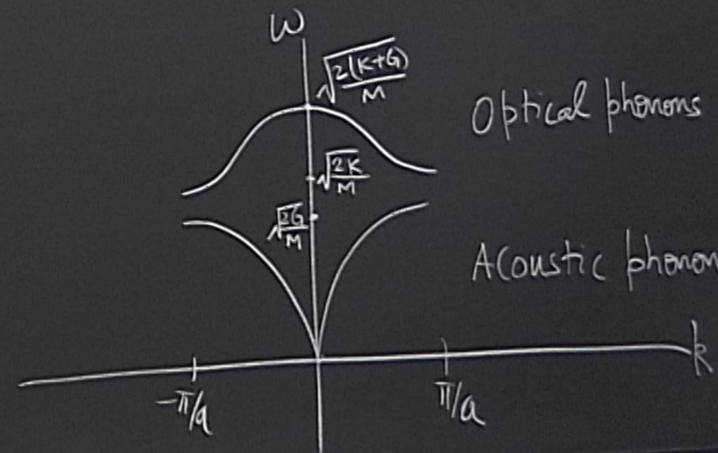
$$u_1(na) = \epsilon_1 e^{i(kna-\omega t)}$$

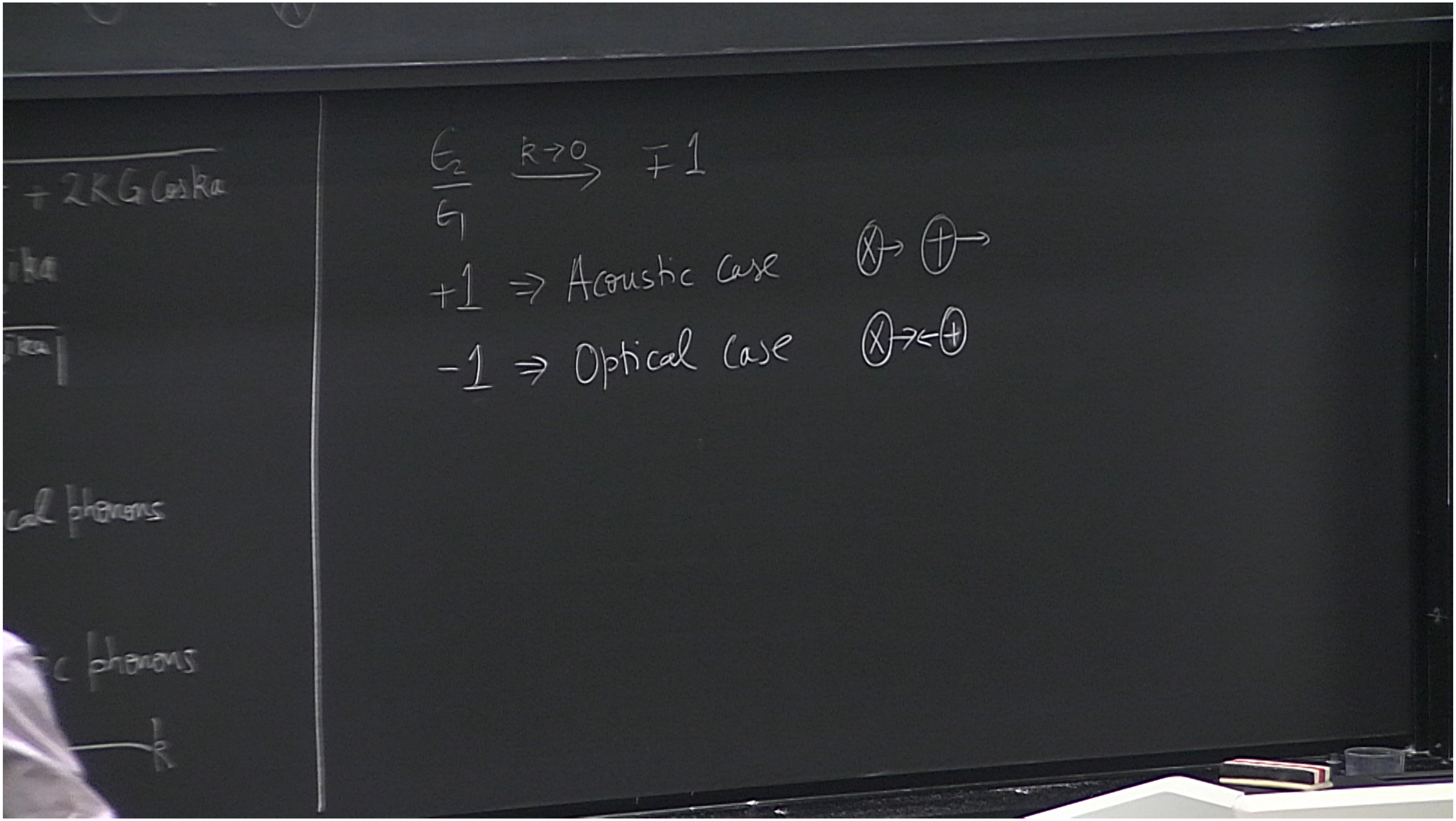
$$u_2(na) = \epsilon_2 e^{i(kna-\omega t)}$$

$$\omega^2 = \frac{K+G}{M} \pm \frac{1}{M}\sqrt{K^2+G^2+2KG\cos ka}$$

and

$$\frac{\epsilon_2}{\epsilon_1} = \mp \frac{K+Ge^{ika}}{|K+Ge^{ika}|}$$




$\frac{G_2}{G_1} \xrightarrow{k\to 0} \mp 1$
$+1 \Rightarrow$ Acoustic case
$-1 \Rightarrow$ Optical case