Title: 14/15 PSI - Condensed Matter-Lecture 6

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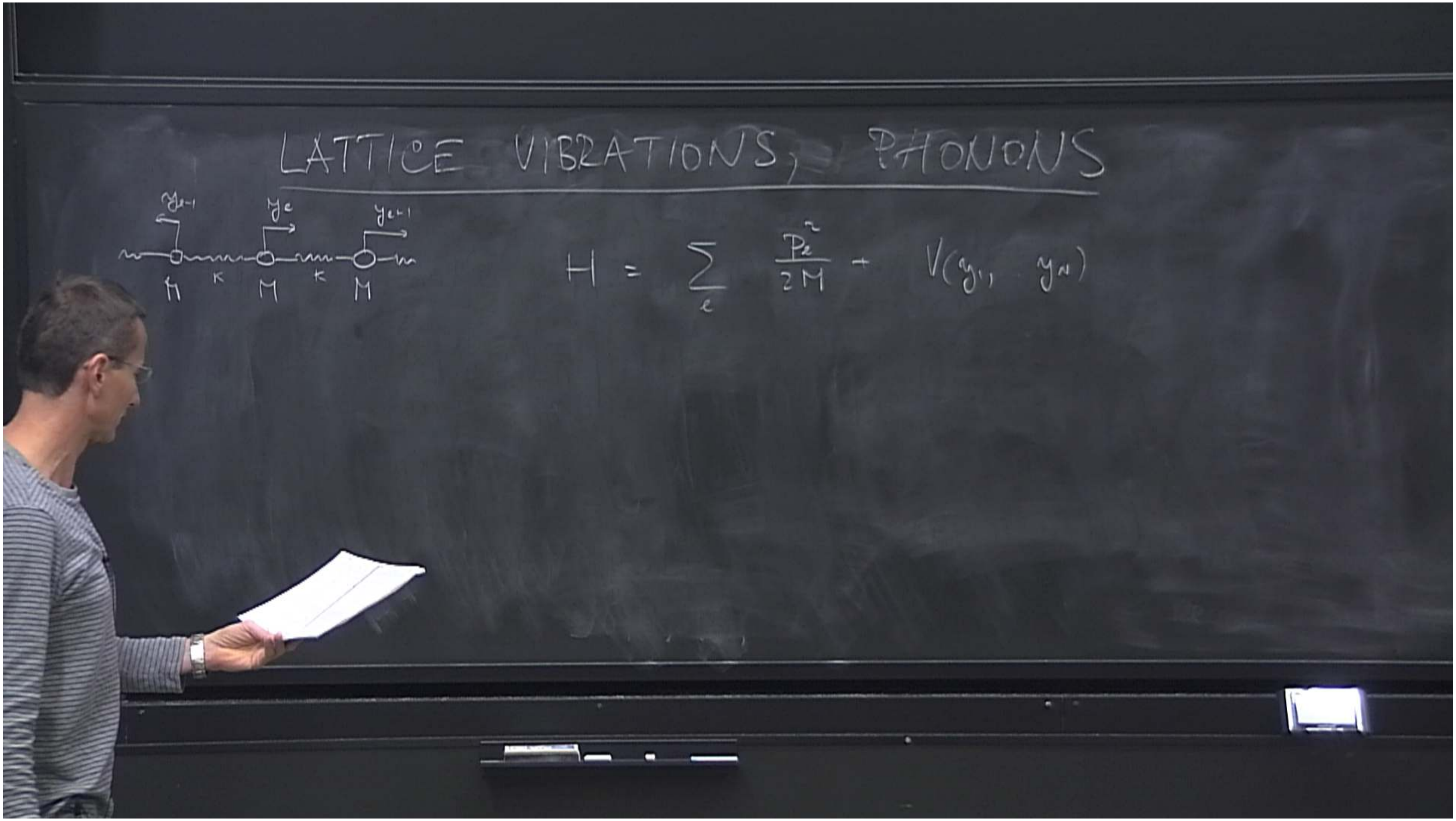
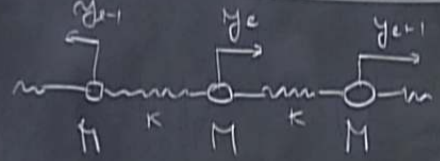
Abstract:


LATTICE VIBRATIONS, PHONONS
$y_{\ell-1}$ y_ℓ $y_{\ell+1}$
M K M K M
$H = \sum_\ell \frac{p_\ell^2}{2M} + V(y_1, \ldots y_N)$

LATTICE VIBRATIONS, PHONONS



$$H = \sum_\ell \frac{p_\ell^2}{2M} + V(y_1, \ldots, y_N)$$

$p_\ell = -i\hbar$

Expand (assuming small displacements):

$$V(y_1 \ldots y_N) = V(0, 0, \ldots 0) + \sum_\ell y_\ell \overbrace{\left[\frac{\partial}{\partial y_\ell} V(y_1 \ldots y_N)\right]_{y_\ell = 0}}^{0}$$

$$+ \frac{1}{2!} \sum_{\ell, \ell'} y_\ell y_{\ell'} \left[\frac{\partial^2}{\partial y_\ell \partial y_{\ell'}} V(y_1 \ldots y_N)\right]_{y_\ell = 0} + O(y_\ell^3)$$

ONS

$\ldots y_N)$

$y_l = 0$

$+ O(y_l^3)$

$$p_l = -i\hbar \frac{\partial}{\partial y_l} \quad \Rightarrow \quad [y_l, p_{l'}] = i\hbar\,\delta_{ll'}$$

In the harmonic approximation: "Dynamical matrix"

$$H = \sum_{l} \frac{p_l^2}{2M} + \sum_{l,l'} y_l y_{l'} V_{ll'}$$

ONS

$y_N)$

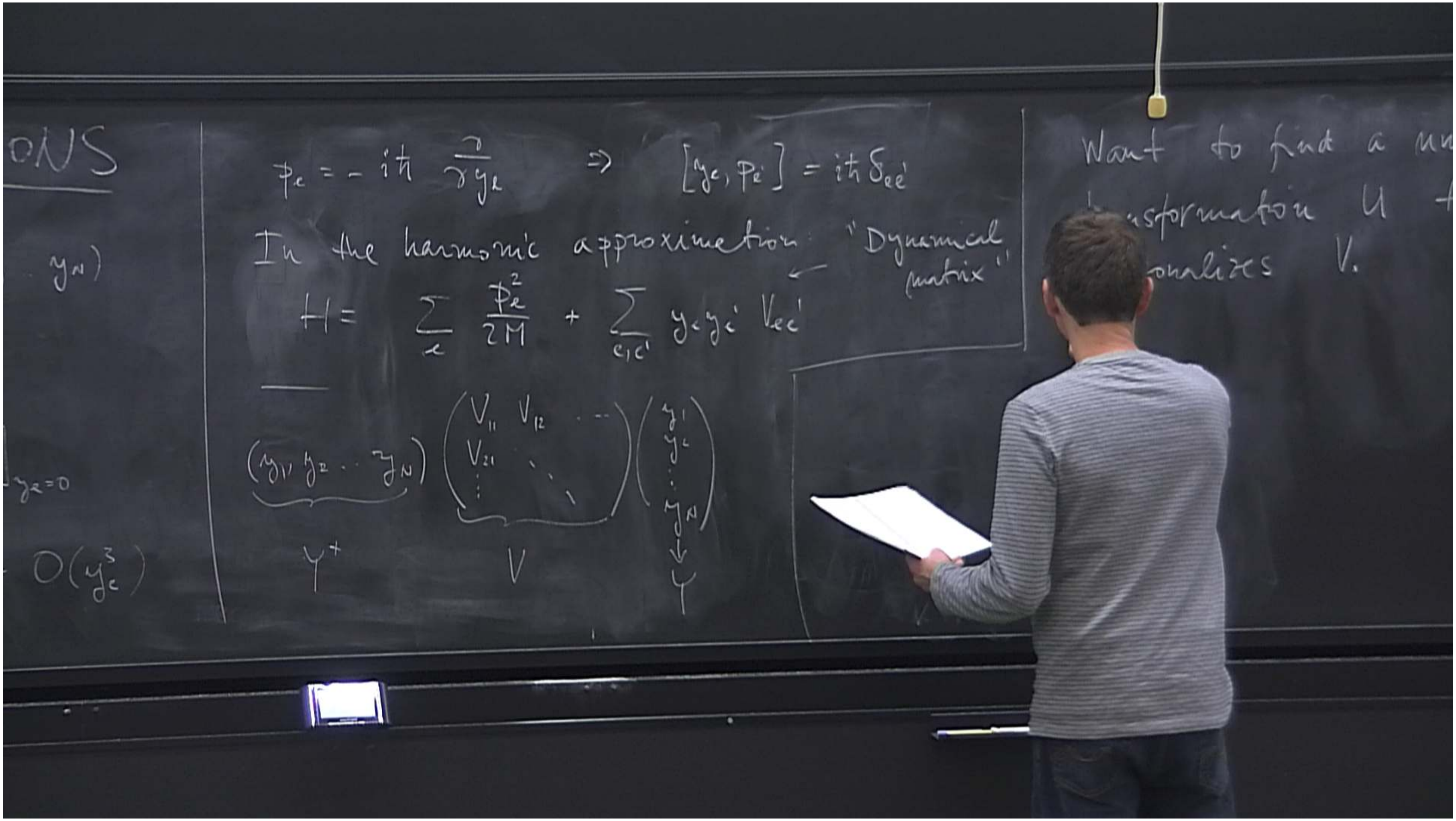
$y_\ell^3)$

$$p_\ell = -i\hbar \frac{\partial}{\partial y_\ell} \Rightarrow [y_\ell, p_{\ell'}] = i\hbar\,\delta_{\ell\ell'}$$

In the harmonic approximation: "Dynamical matrix"

$$H = \sum_\ell \frac{p_\ell^2}{2M} + \sum_{\ell,\ell'} y_\ell y_{\ell'} V_{\ell\ell'}$$

$$(y_1, y_2 \cdots y_N) \begin{pmatrix} V_{11} & V_{12} & \cdots \\ V_{21} & \ddots & \\ \vdots & & \ddots \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}$$


ONS
$p_\ell = -i\hbar \frac{\partial}{\partial y_\ell} \Rightarrow [y_\ell, p_{\ell'}] = i\hbar\delta_{\ell\ell'}$
In the harmonic approximation:
"Dynamical matrix"
$H = \sum_\ell \frac{p_\ell^2}{2M} + \sum_{\ell,\ell'} y_\ell y_{\ell'} V_{\ell\ell'}$
$\underbrace{(y_1, y_2 \cdots y_N)}_{Y^+} \underbrace{\begin{pmatrix} V_{11} & V_{12} & \cdots \\ V_{21} & \ddots & \\ \vdots & & \ddots \end{pmatrix}}_{V} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} \rightarrow Y$
$O(y_\ell^3)$
Want to find a un
transformation U t
onalizes V.

$\Rightarrow \quad [y_\ell, p_{\ell'}] = i\hbar\, \delta_{\ell\ell'}$

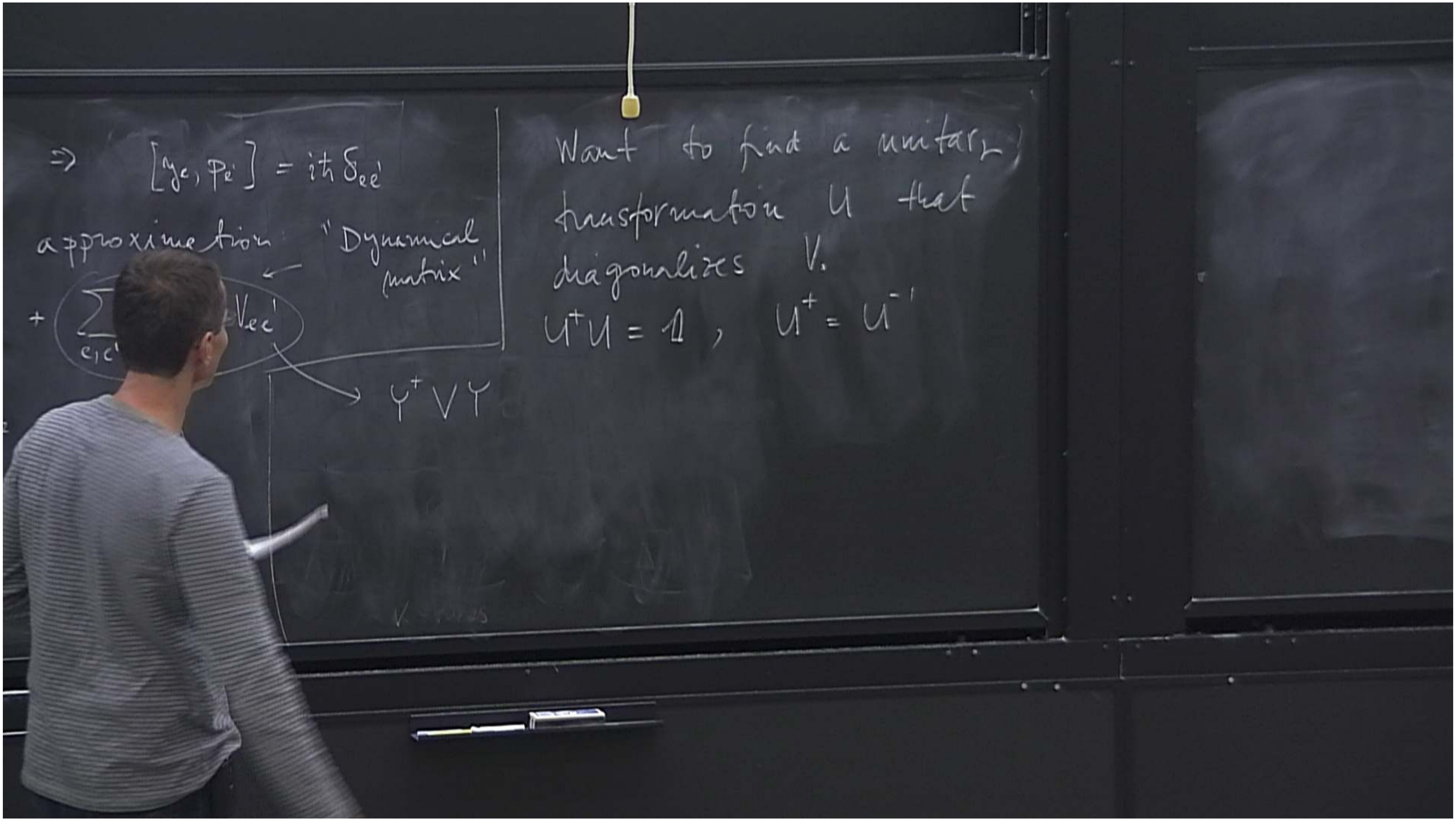
approximation ← "Dynamical matrix"

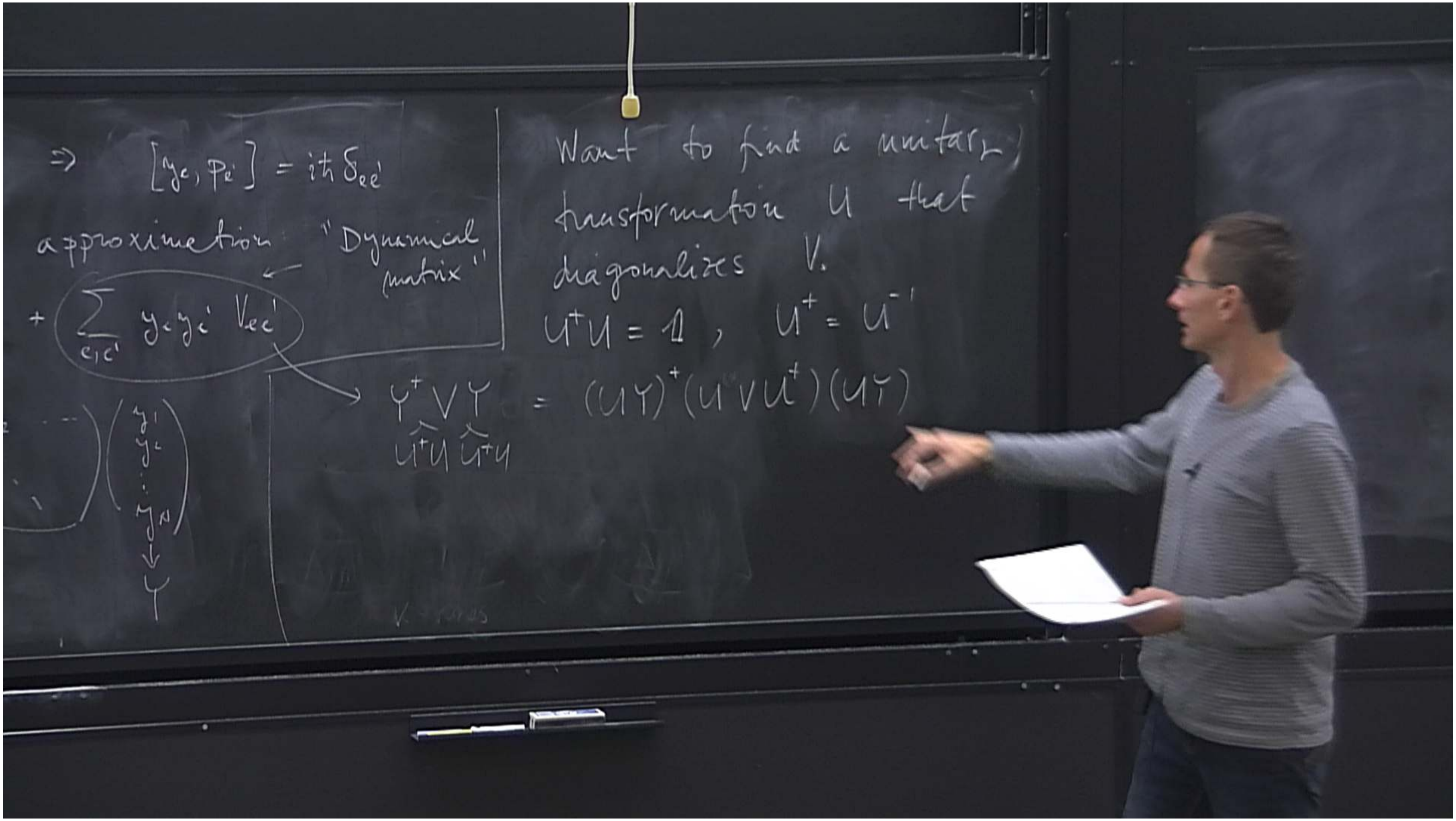
$+ \sum_{\ell,\ell'} y_\ell y_{\ell'} V_{\ell\ell'}$

$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} \to Y$

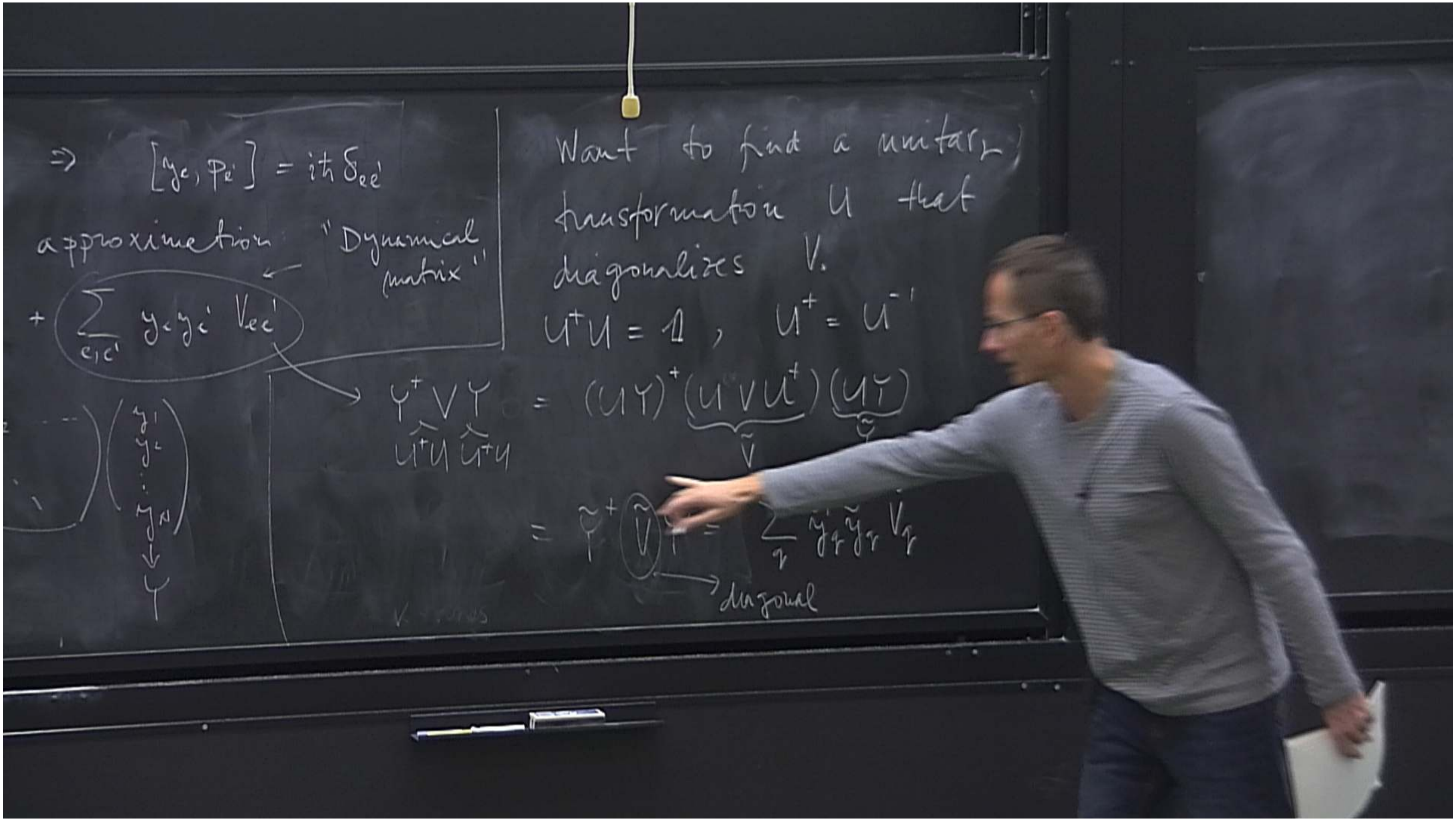
Want to find a unitary transformation U that diagonalizes V.

$U^\dagger U = \mathbb{1}, \quad U^\dagger = U^{-1}$


⇒ $[y_e, p_{e'}] = i\hbar\,\delta_{ee'}$
approximation
"Dynamical matrix"
$+ \sum_{e,e'} V_{ee'}$
$Y^+ V Y$
Want to find a unitary transformation U that diagonalizes V.
$U^+U = 1, \quad U^+ = U^{-1}$



Want to find a unitary transformation U that diagonalizes V.
U⁺U = 1 , U⁺ = U⁻¹
approximation
"Dynamical matrix"


$\Rightarrow \quad [y_c, p_{c'}] = i\hbar\,\delta_{cc'}$
approximation
"Dynamical matrix"
$+ \sum_{c,c'} y_c y_{c'} V_{cc'}$
Want to find a unitary transformation U that diagonalizes V.
$U^+U = \mathbb{1}, \quad U^+ = U^{-1}$
$Y^+ V Y = (UY)^+ (UVU^+)(UY)$
$= \tilde{Y}^+ \tilde{V} \tilde{Y} = \sum_q \tilde{y}_q \tilde{y}_q V_q$
diagonal

$p_\ell = -i\hbar \frac{\partial}{\partial y_\ell} \Rightarrow [y_\ell, p_{\ell'}] = i\hbar\,\delta_{\ell\ell'}$

In the harmonic approximation ← "Dynamical matrix"

$$H = \sum_\ell \frac{p_\ell^2}{2M} + \sum_{\ell,\ell'} y_\ell y_{\ell'} V_{\ell\ell'}$$

$$\underbrace{(y_1, y_2 \cdots y_N)}_{Y^+} \underbrace{\begin{pmatrix} V_{11} & V_{12} & \cdots \\ V_{21} & \ddots & \\ \vdots & & \ddots \end{pmatrix}}_{V} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} \to Y$$

Want to find a unitary transformation U that diagonalizes V.

$U^+U = \mathbb{1}, \quad U^+ = U^{-1}$

$$Y^+ \overbrace{\ }^{U^+U} V \overbrace{\ }^{U^+U} Y = (UY)^+ \underbrace{(UVU^+)}_{\tilde{V}} \underbrace{(UY)}_{\tilde{Y}}$$

$$= \tilde{Y}^+ \tilde{V} \tilde{Y} = \sum_q \tilde{y}_q^+ \tilde{y}_q \tilde{V}_q$$

$\tilde{V}$ → diagonal

$$p_\ell = -i\hbar \frac{\partial}{\partial y_\ell} \Rightarrow [y_\ell, p_{\ell'}] = i\hbar\,\delta_{\ell\ell'}$$

In the harmonic approximation: "Dynamical matrix"

$$H = \sum_\ell \frac{p_\ell^2}{2M} + \sum_{\ell,\ell'} y_\ell y_{\ell'} V_{\ell\ell'}$$

$$\underbrace{(y_1, y_2 \cdots y_N)}_{Y^+} \underbrace{\begin{pmatrix} V_{11} & V_{12} & \cdots \\ V_{21} & \ddots & \\ \vdots & & \ddots \end{pmatrix}}_{V} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} \to Y$$

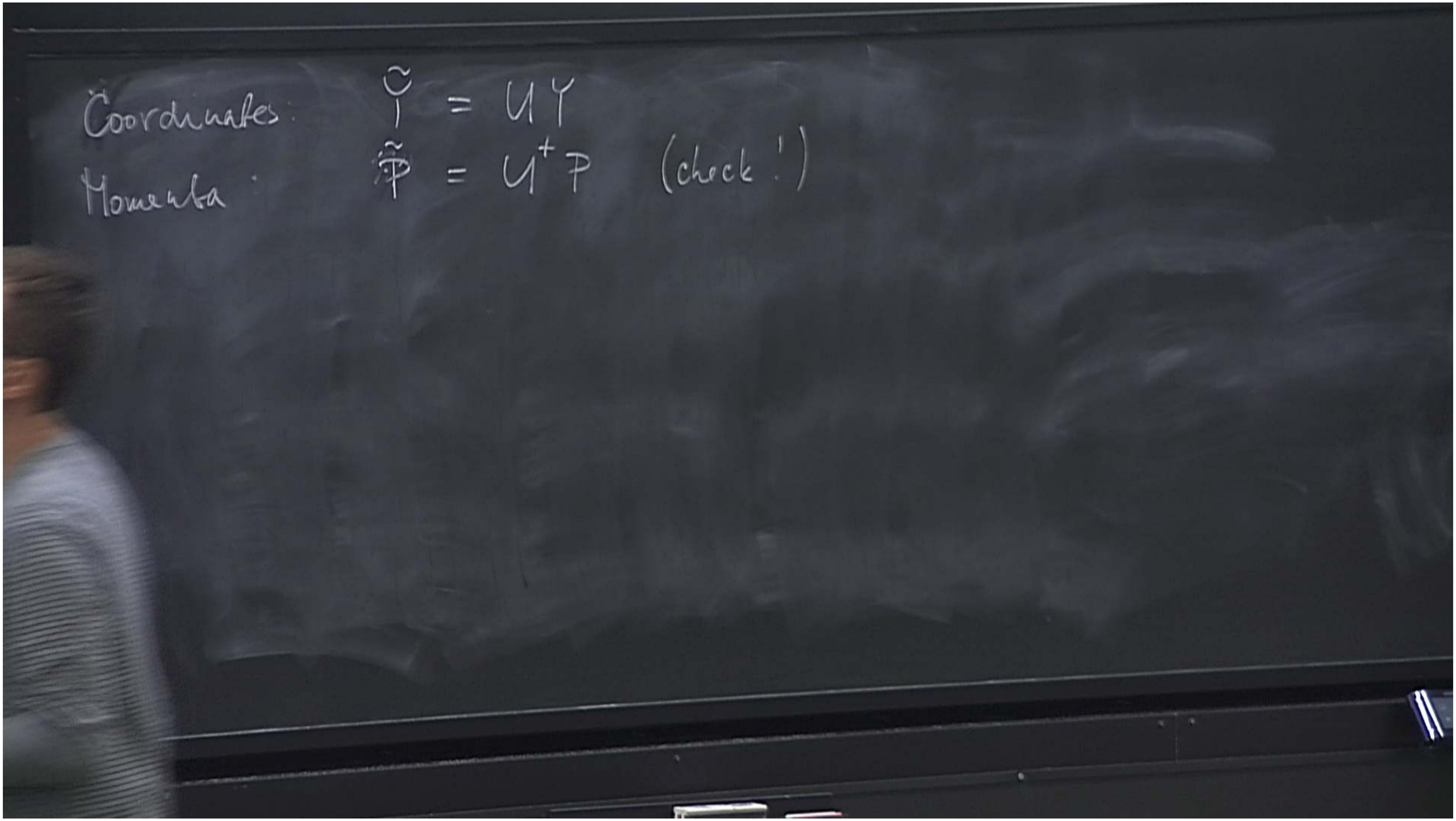
Want to find a unitary transformation U that diagonalizes V.

$$U^+U = \mathbb{1}, \quad U^+ = U^{-1}$$

$$Y^+ \overbrace{U^+U}\, V \overbrace{U^+U}\, Y = (UY)^+ \underbrace{(UVU^+)}_{\tilde{V}} \underbrace{(UY)}_{\tilde{Y}}$$

$$= \tilde{Y}^+ \tilde{V} \tilde{Y} = \sum_q \tilde{y}_q^+ \tilde{y}_q \tilde{V}_q$$

$\tilde{V} \to$ diagonal


Coordinates: $\tilde{Y} = U Y$
Momenta: $\tilde{P} = U^{+} P$ (check!)

Coordinates: $\tilde{Y} = U Y$

Momenta: $\tilde{P} = U^{+} P$ (check!)

$\Rightarrow [\tilde{y}_q, \tilde{p}_{q'}] = i\hbar\,\delta_{qq'}$ (check!)

Coordinates: $\tilde{y} = U y$

Momenta: $\tilde{p} = U^{+} p$ (check!)

$\Rightarrow [\tilde{y}_q, \tilde{p}_{q'}] = i\hbar\,\delta_{qq'}$ (check!)

$$H = \sum_q \left(\frac{1}{2M} \tilde{p}_q^{+} \tilde{p}_q + \frac{1}{2} M \omega_q^2 \tilde{y}_q^{+} \tilde{y}_q \right)$$

$\omega_q = \sqrt{\frac{V_q}{M}}$ – "phonon frequencies"

collection of indep. harmonic oscillators.

Define raising & lo

P (check!)

(check!)

$\omega_q^2 \tilde{y}_q^+ \tilde{y}_q)$

quencies"

onic

lators.

Define raising & lowering operators for each LHO.

$$a_q = \frac{1}{\sqrt{2M\hbar\omega_q}}\left(M\omega_q \tilde{y}_q + i\tilde{p}_q^+\right)$$

$$a_q^+ = \frac{1}{\sqrt{2M\hbar\omega_q}}\left(M\omega_q \tilde{y}_q^+ - i\tilde{p}_q\right)$$

$$\boxed{H = \sum_q \hbar\omega_q\left(a_q^+ a_q + \frac{1}{2}\right)}$$

(check!)

(check!)

$\omega_q^2 \tilde{y}_q^+ \tilde{y}_q)$

quencies"

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lators.

Define raising & lowering operators for each LHO.

$$a_q = \frac{1}{\sqrt{2M\hbar\omega_q}}\left(M\omega_q \tilde{y}_q + i\tilde{p}_q^+\right)$$

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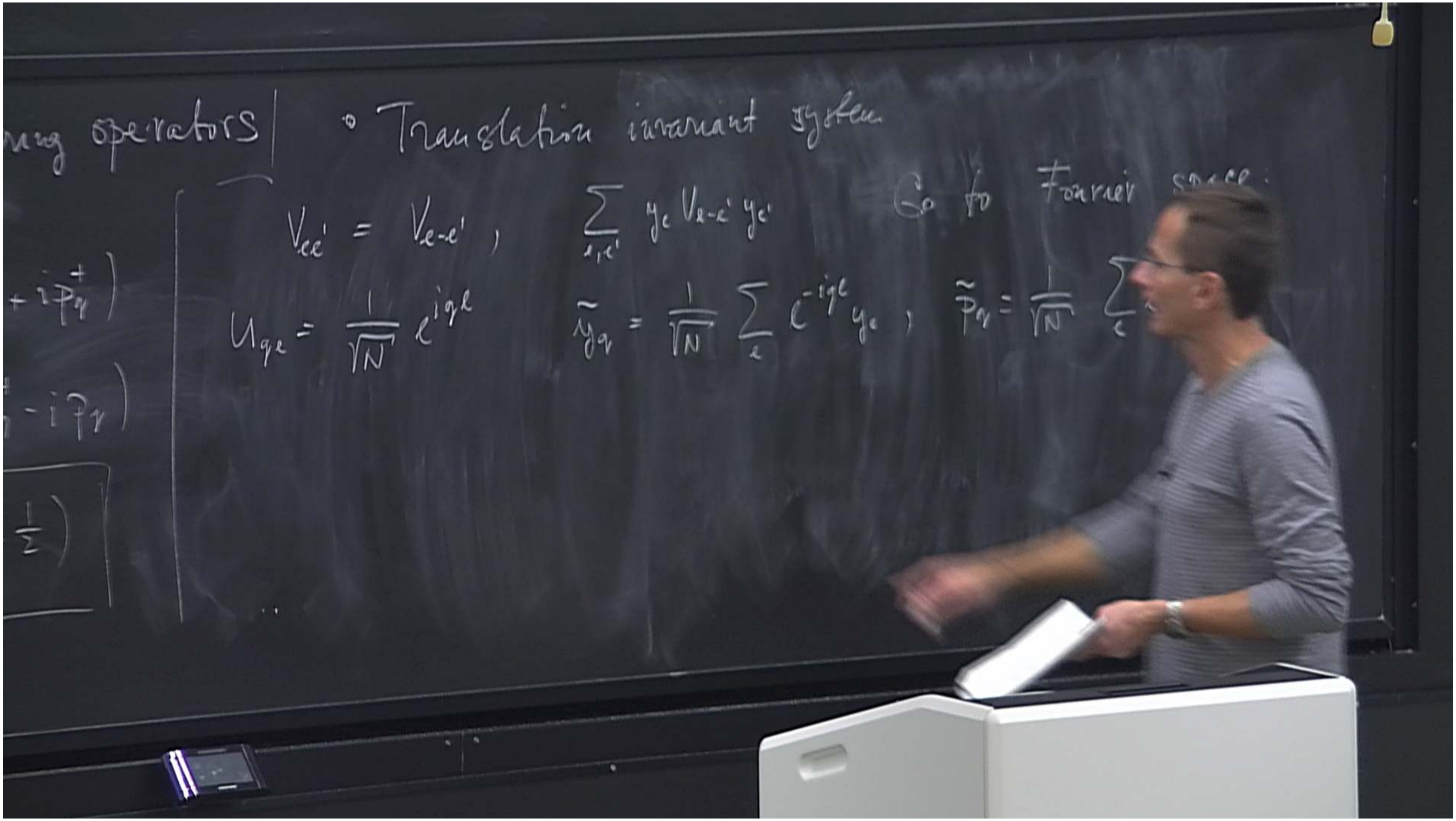
$$\boxed{H = \sum_q \hbar\omega_q\left(a_q^+ a_q + \frac{1}{2}\right)}$$


operators
• Translation invariant system
Go to Fourier space
$V_{\ell\ell'} = V_{\ell-\ell'}$, $\sum_{\ell,\ell'} y_\ell V_{\ell-\ell'} y_{\ell'}$
$U_{q\ell} = \frac{1}{\sqrt{N}} e^{iq\ell}$
$\tilde{y}_q = \frac{1}{\sqrt{N}} \sum_\ell e^{-iq\ell} y_\ell$, $\tilde{p}_q = \frac{1}{\sqrt{N}} \sum_\ell$

ing operators

$+ i\tilde{p}_q^\dagger)$

$- i\tilde{p}_q)$

$\frac{1}{2})$

• Translation invariant system

$V_{\ell\ell'} = V_{\ell-\ell'}$, $\sum_{\ell,\ell'} y_\ell V_{\ell-\ell'} y_{\ell'}$ Go to Fourier space:

$U_{q\ell} = \frac{1}{\sqrt{N}} e^{iq\ell}$ $\tilde{y}_q = \frac{1}{\sqrt{N}} \sum_\ell e^{-iq\ell} y_\ell$, $\tilde{p}_q = \frac{1}{\sqrt{N}} \sum_\ell e^{+iq\ell} p_\ell$

• Use periodic b.c.: $y_{\ell+Na} = y_\ell$

...

...ing operators | ◦ Translation invariant system

$(\ldots + i\tilde{p}_q^+)$

$(\ldots - i\tilde{p}_q)$

$\left(\frac{1}{2}\right)$

$V_{\ell\ell'} = V_{\ell-\ell'}$, $\sum_{\ell,\ell'} y_\ell V_{\ell-\ell'} y_{\ell'}$ Go to Fourier space:

$U_{q\ell} = \frac{1}{\sqrt{N}} e^{iq\ell}$ $\tilde{y}_q = \frac{1}{\sqrt{N}} \sum_\ell e^{-iq\ell} y_\ell$, $\tilde{p}_q = \frac{1}{\sqrt{N}} \sum_\ell e^{+iq\ell} p_\ell$

◦ Use periodic b.c.: $y_{\ell+Na} = y_\ell$

$e^{iq\ell} = e^{iq(\ell+Na)}$

...

- Use periodic b.c.: $y_{\ell+Na} = y_\ell$

$e^{iq\ell} = e^{iq(\ell+Na)}$

$1 = e^{iqNa}$

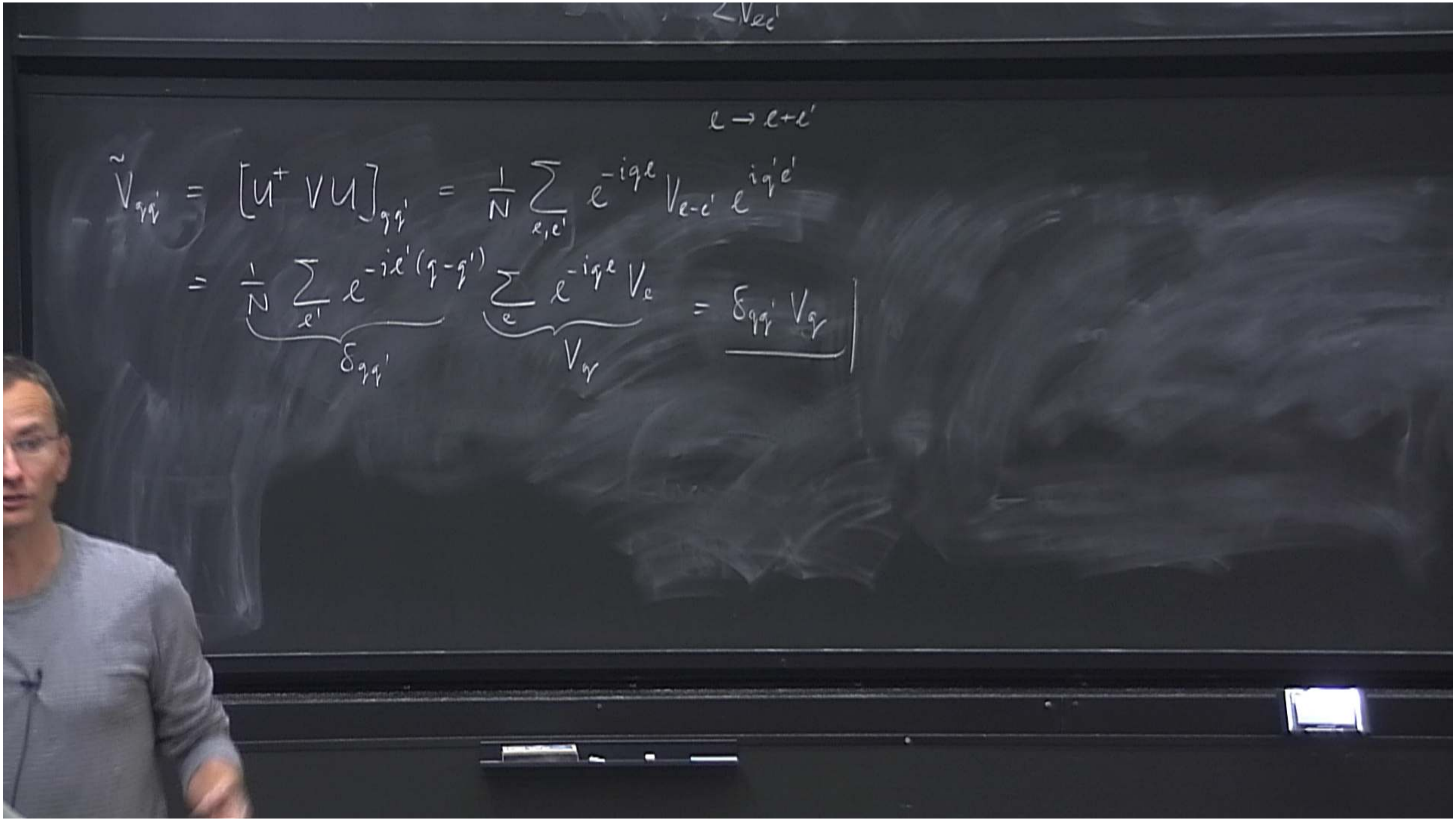
$q = \frac{2\pi}{a}\frac{n}{N}, \quad n \in \mathbb{Z}$

$y_q = y_{q+G}, \quad p_q = p_{q+G}$

$G = \frac{2\pi}{a}$

Reciprocal lattice vector

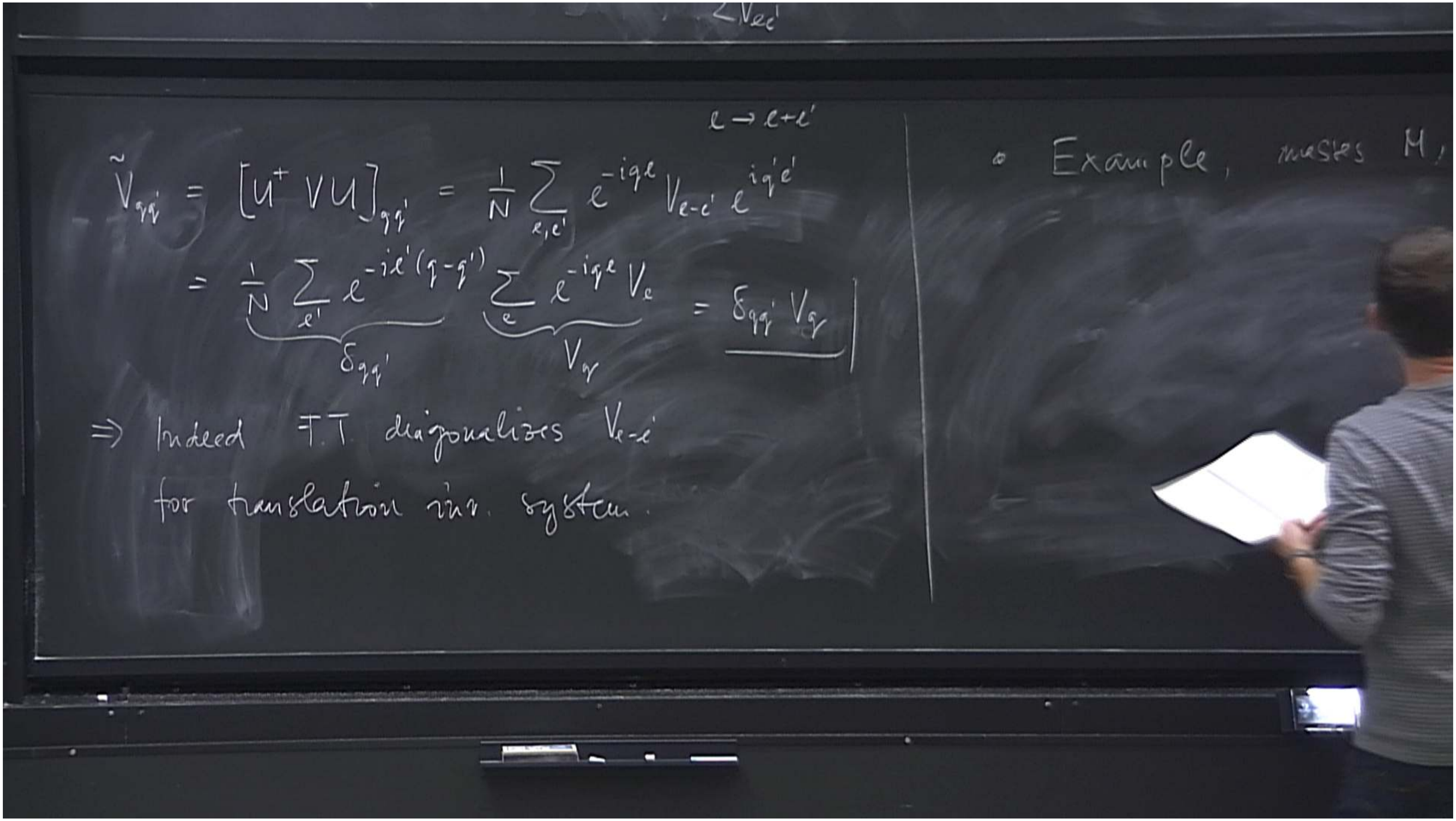
$q \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right)$


$\ell \to \ell + \ell'$
$\tilde{V}_{qq'} = [U^+ V U]_{qq'} = \frac{1}{N}\sum_{\ell,\ell'} e^{-iq\ell} V_{\ell-\ell'} e^{iq'\ell'}$
$= \underbrace{\frac{1}{N}\sum_{\ell'} e^{-i\ell'(q-q')}}_{\delta_{qq'}} \underbrace{\sum_{\ell} e^{-iq\ell} V_{\ell}}_{V_q} = \boxed{\delta_{qq'} V_q}$

$$\ell \to \ell + \ell'$$

$$\tilde{V}_{qq'} = [U^{+} V U]_{qq'} = \frac{1}{N}\sum_{\ell,\ell'} e^{-iq\ell} V_{\ell-\ell'} e^{iq'\ell'}$$

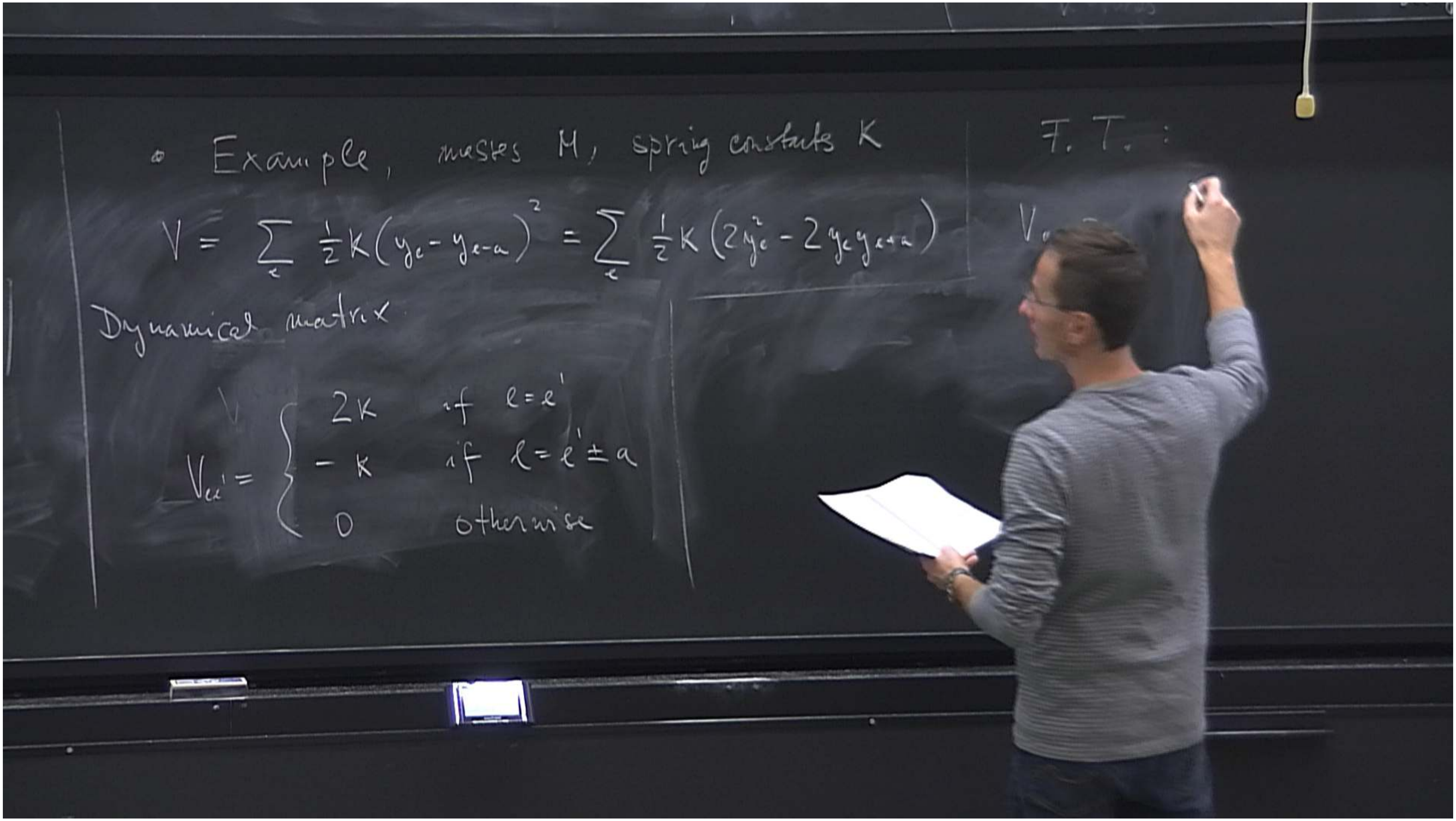
$$= \underbrace{\frac{1}{N}\sum_{\ell'} e^{-i\ell'(q-q')}}_{\delta_{qq'}} \underbrace{\sum_{\ell} e^{-iq\ell} V_{\ell}}_{V_q} = \underline{\delta_{qq'} V_q}$$


$\sum V_{\ell\ell'}$
$\ell \to \ell+\ell'$
$\tilde{V}_{qq'} = [U^\dagger V U]_{qq'} = \frac{1}{N}\sum_{\ell,\ell'} e^{-iq\ell} V_{\ell-\ell'} e^{iq'\ell'}$
$= \underbrace{\frac{1}{N}\sum_{\ell'} e^{-i\ell'(q-q')}}_{\delta_{qq'}} \underbrace{\sum_{\ell} e^{-iq\ell} V_\ell}_{V_q} = \boxed{\delta_{qq'} V_q}$
$\Rightarrow$ Indeed F.T. diagonalizes $V_{\ell-\ell'}$
for translation inv. system.
• Example, masses M,

- Example, masses M, spring constants K

- Example, masses M, spring constants K

$$V = \sum_{\ell} \frac{1}{2} K \left(y_\ell - y_{\ell-a} \right)^2 = \sum_{\ell} \frac{1}{2} K \left(2 y_\ell^2 - 2 y_\ell y_{\ell+a} \right)$$



• Example, masses M, spring constants K
$V = \sum_l \frac{1}{2}K(y_l - y_{l-a})^2 = \sum_l \frac{1}{2}K(2y_l^2 - 2y_l y_{l+a})$
Dynamical matrix
$V_{ll'} = \begin{cases} 2K & \text{if } l = l' \\ -K & \text{if } l = l' \pm a \\ 0 & \text{otherwise} \end{cases}$
F. T.:

• Example, masses M, spring constants K

$$V = \sum_\ell \tfrac{1}{2}K(y_\ell - y_{\ell-a})^2 = \sum_\ell \tfrac{1}{2}K(2y_\ell^2 - 2y_\ell y_{\ell+a})$$

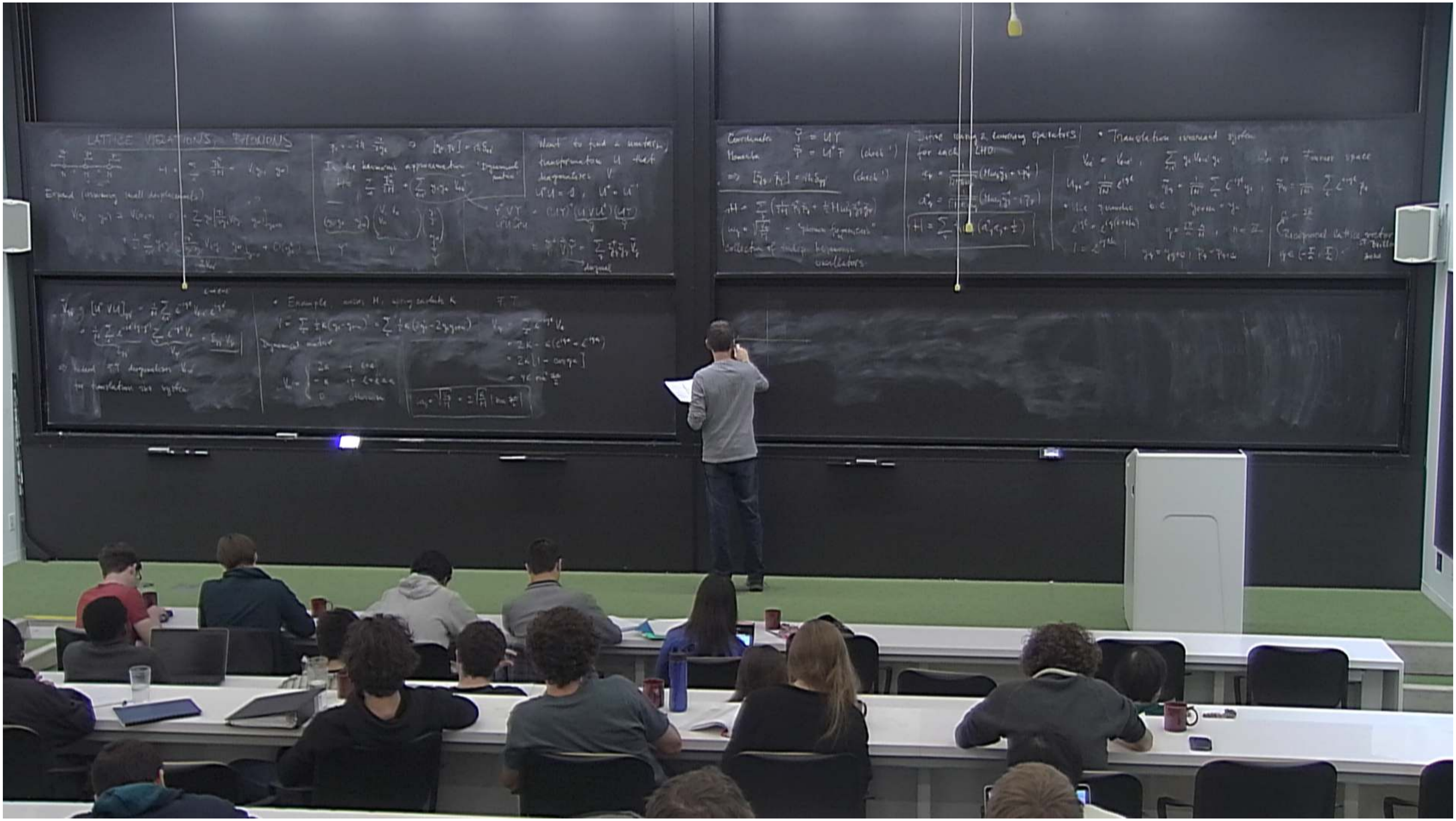
Dynamical matrix

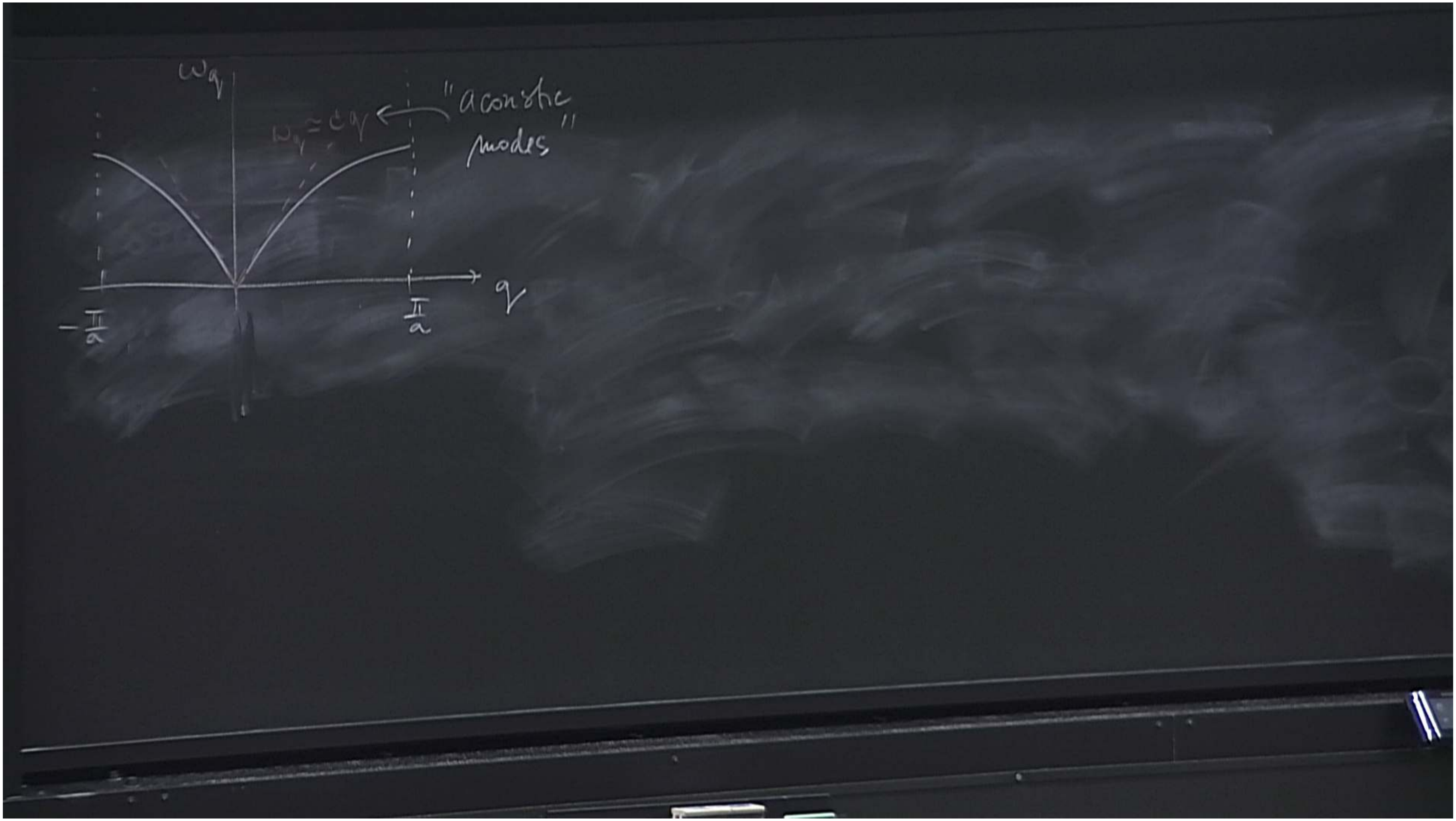
$$V_{\ell\ell'} = \begin{cases} 2K & \text{if } \ell = \ell' \\ -K & \text{if } \ell = \ell' \pm a \\ 0 & \text{otherwise} \end{cases}$$

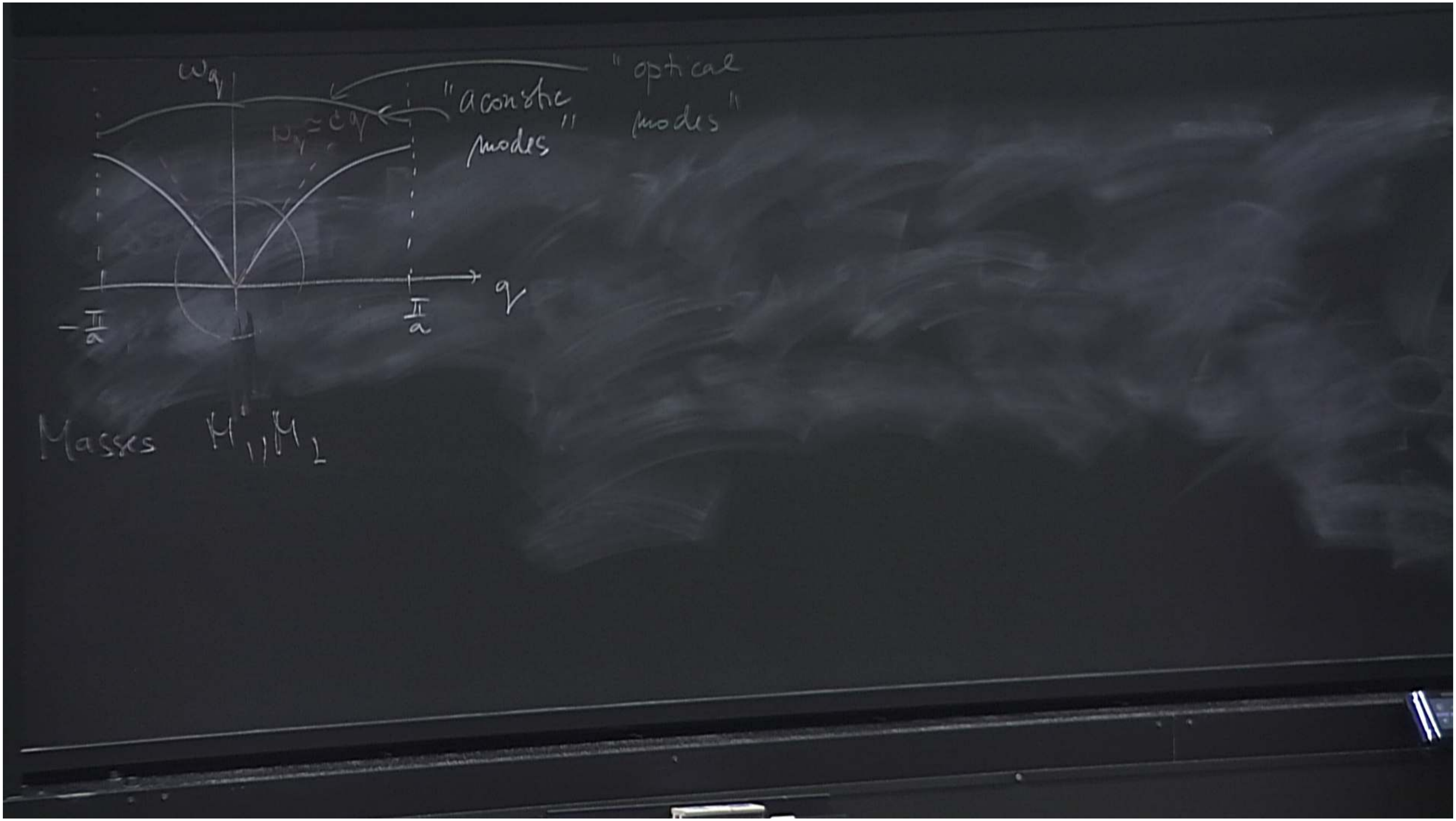
F.T.:

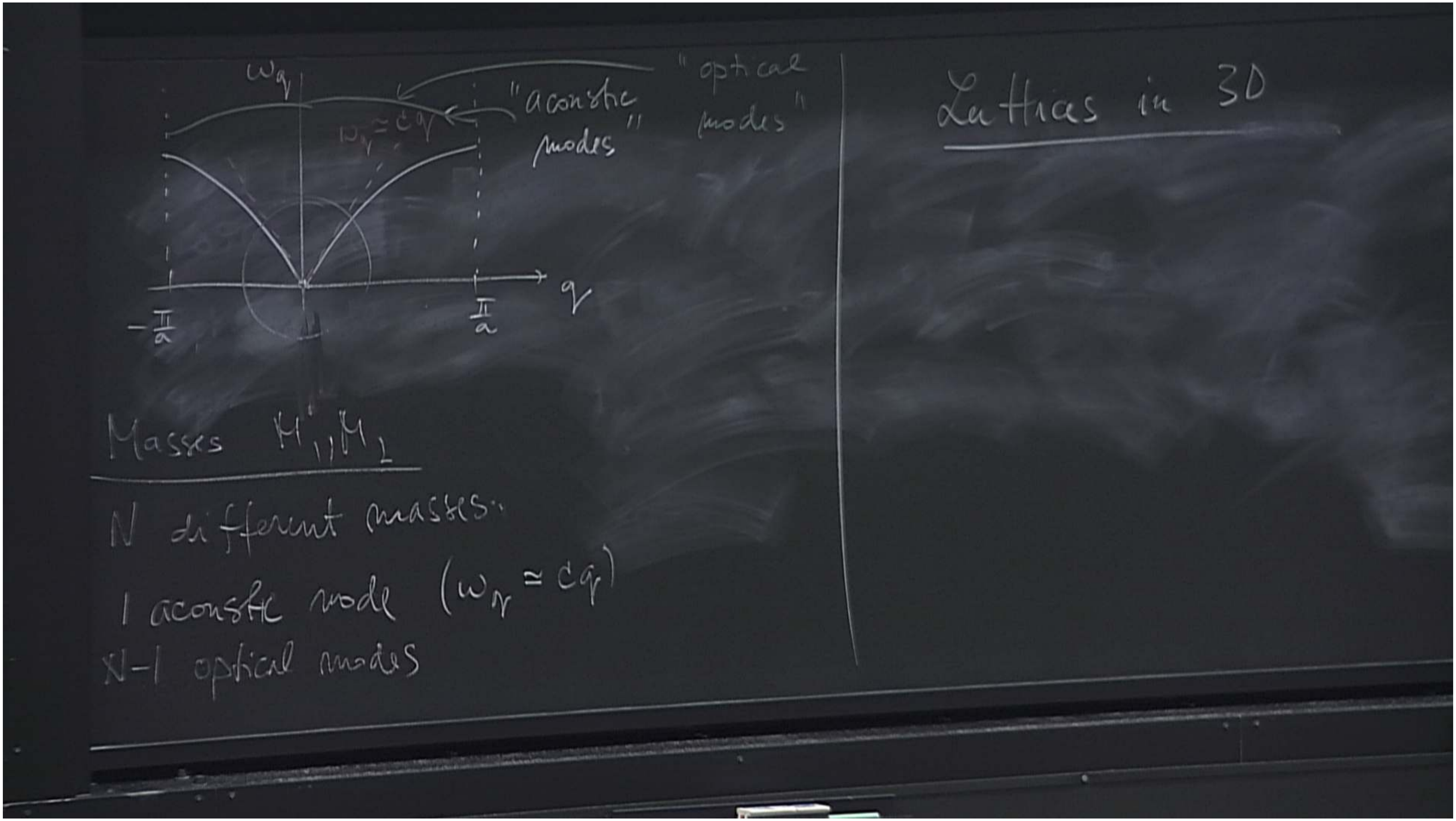
$$V_q = \sum_\ell e^{-iq\ell} V_\ell$$
$$= 2K - K(e^{iqa} + e^{-iqa})$$
$$= 2K[1 - \cos qa]$$
$$= 4K \sin^2 \frac{qa}{2}$$

$$\boxed{\omega_q = \sqrt{\frac{V_q}{M}} = 2\sqrt{\frac{K}{M}}\left|\sin\frac{qa}{2}\right|}$$

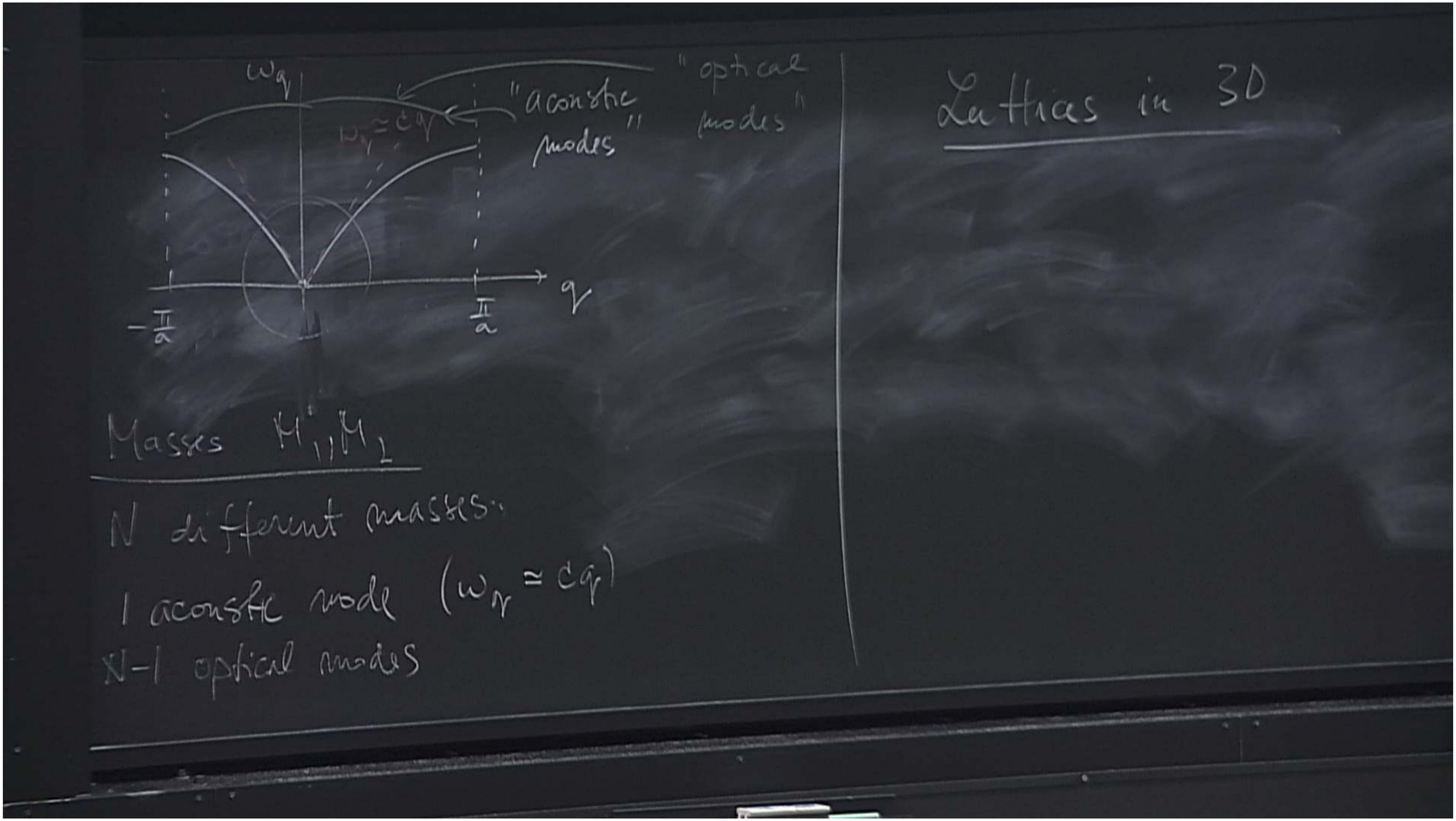


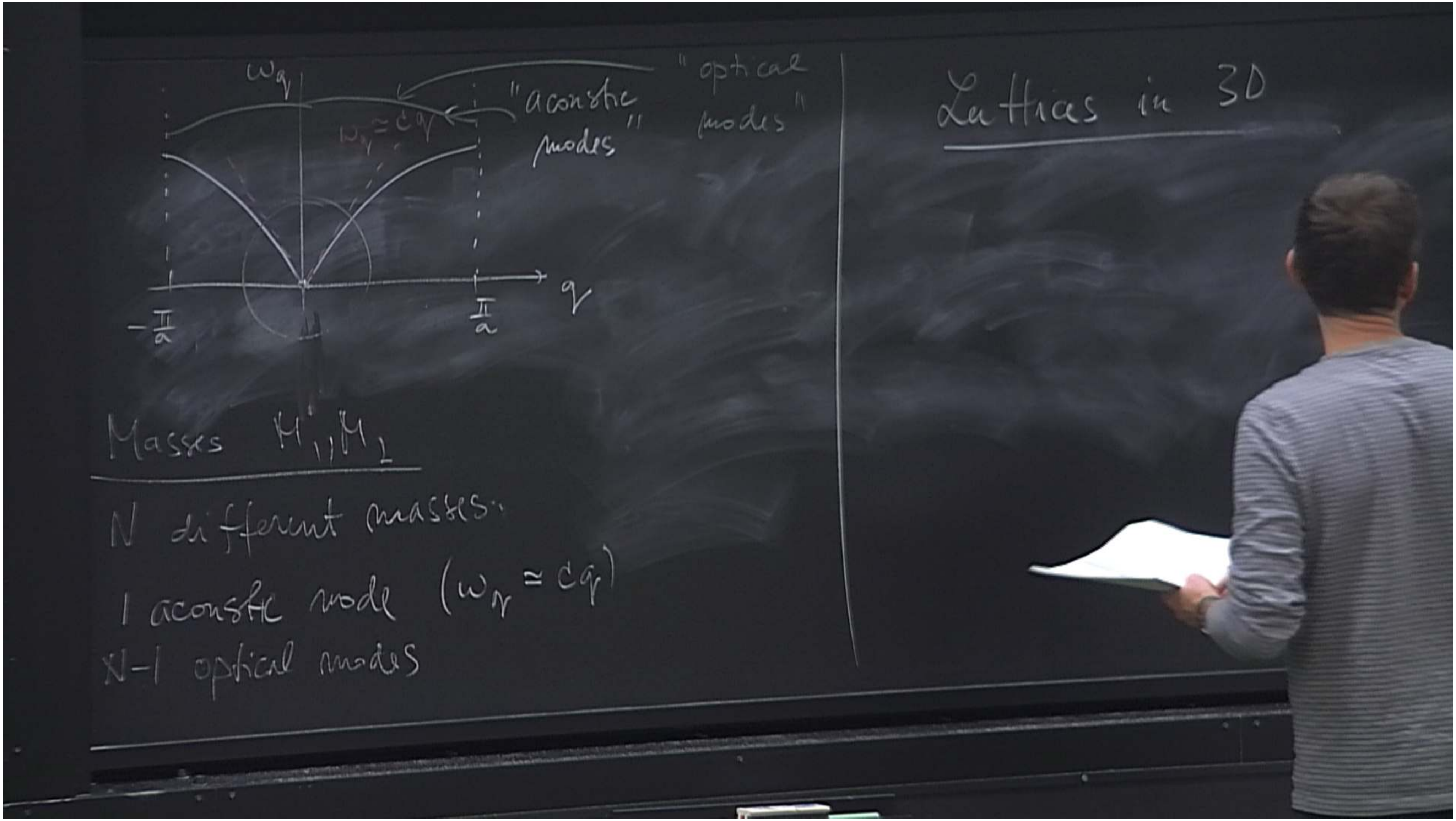

ω_q
$\omega_q \simeq cq$
"acoustic modes"
q
$-\frac{\pi}{a}$
$\frac{\pi}{a}$


ω_q
"optical modes"
"acoustic modes"
$\omega_q \simeq c q$
q
$-\frac{\pi}{a}$
$\frac{\pi}{a}$
Masses M_1, M_2



ω_q
$\omega_q \simeq cq$
"acoustic modes"
"optical modes"
q
$-\frac{\pi}{a}$
$\frac{\pi}{a}$
Masses M_1, M_2
N different masses:
1 acoustic mode ($\omega_q \simeq cq$)
N-1 optical modes
Lattices in 3D


"optical modes"
"acoustic modes"
ω_q
$\omega_q \simeq cq$
q
$-\frac{\pi}{a}$
$\frac{\pi}{a}$
Masses M_1, M_2
N different masses:
1 acoustic mode ($\omega_q \simeq cq$)
N−1 optical modes
Lattices in 3D



ω_q
"optical modes"
"acoustic modes"
$\omega_q \simeq cq$
q
$-\frac{\pi}{a}$
$\frac{\pi}{a}$
Lattices in 3D
Masses M_1, M_2
N different masses:
1 acoustic mode ($\omega_q \simeq cq$)
N−1 optical modes

Lattices in 3D

$$\vec{l} = n_1 \vec{l}_1 + n_2 \vec{l}_2 + n_3 \vec{l}_3$$

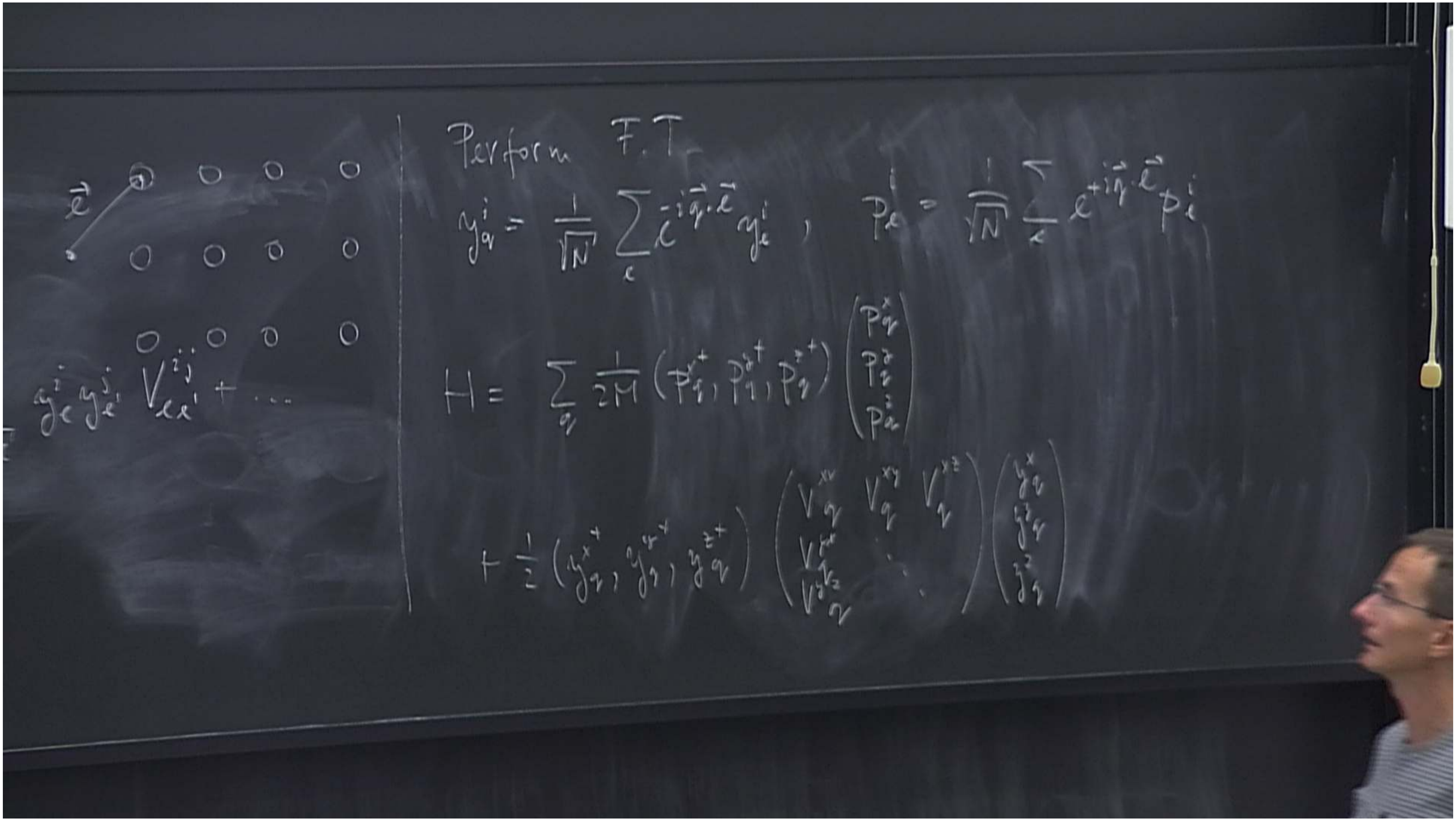
$$H = \sum_{\vec{l}, i} \frac{(p^i_{\vec{l}})^2}{2M} + \frac{1}{2} \sum_{\substack{l, l' \\ i, j}} y^i_l y^j_{l'} V^{ij}_{l l'} + \dots$$

$i, j = x, y, z$

$$V^{ij}_{l l'} = \frac{\partial^2 V}{\partial y^i_l \, \partial y^j_{l'}}$$

Perform F.T.

$$y^i_q = \frac{1}{\sqrt{N}} \sum_l e^{-i \vec{q} \cdot \vec{l}} y^i_l \,, \quad p^i_l =$$



$\vec{\ell}$
$y^i_\ell \, y^j_{\ell'} \, V^{ij}_{\ell\ell'} + \dots$
Perform F.T.
$y^i_q = \frac{1}{\sqrt{N}} \sum_\ell e^{-i\vec{q}\cdot\vec{\ell}} y^i_\ell \,, \quad p^i_\ell = \frac{1}{\sqrt{N}} \sum_\ell e^{+i\vec{q}\cdot\vec{\ell}} p^i_\ell$
$H = \sum_q \frac{1}{2M} \left(p^{x+}_q, p^{y+}_q, p^{z+}_q\right) \begin{pmatrix} p^x_q \\ p^y_q \\ p^z_q \end{pmatrix}$
$+ \frac{1}{2} \left(y^{x+}_q, y^{y+}_q, y^{z+}_q\right) \begin{pmatrix} V^{xx}_q & V^{xy}_q & V^{xz}_q \\ V^{yx}_q & \ddots & \\ V^{zx}_q & & \ddots \end{pmatrix} \begin{pmatrix} y^x_q \\ y^y_q \\ y^z_q \end{pmatrix}$

$y^i_\ell y^j_{\ell'} V^{ij}_{\ell\ell'} + \dots$

Perform F.T

$$y^i_q = \frac{1}{\sqrt{N}} \sum_\ell e^{-i\vec{q}\cdot\vec{\ell}} y^i_\ell \,, \quad p^i_\ell = \frac{1}{\sqrt{N}} \sum_\ell e^{+i\vec{q}\cdot\vec{\ell}} p^i_\ell$$

$$H = \sum_q \frac{1}{2M} \left(p^{x+}_q, p^{y+}_q, p^{z+}_q\right) \begin{pmatrix} p^x_q \\ p^y_q \\ p^z_q \end{pmatrix}$$

$$+ \frac{1}{2} \left(y^{x+}_q, y^{y+}_q, y^{z+}_q\right) \begin{pmatrix} V^{xx}_q & V^{xy}_q & V^{xz}_q \\ V^{yx}_q & \cdot & \\ V^{zx}_q & & \cdot \end{pmatrix} \begin{pmatrix} y^x_q \\ y^y_q \\ y^z_q \end{pmatrix}$$

3x3 Hermitian Matrix

3 eigenvalues V^1_q, V^2_q, V^3_q

$$y^i_l y^j_{l'} V^{ij}_{ll'} + \dots$$

Perform F.T.

$$y^i_q = \frac{1}{\sqrt{N}} \sum_l e^{-i\vec{q}\cdot\vec{l}}\, y^i_l \,, \qquad p^i_l = \frac{1}{\sqrt{N}} \sum_q e^{+i\vec{q}\cdot\vec{l}}\, p^i_q$$

$$H = \sum_q \frac{1}{2M} \left(p^{x+}_q, p^{y+}_q, p^{z+}_q\right) \begin{pmatrix} p^x_q \\ p^y_q \\ p^z_q \end{pmatrix} + \frac{1}{2} \left(y^{x+}_q, y^{y+}_q, y^{z+}_q\right) \begin{pmatrix} V^{xx}_q & V^{xy}_q & V^{xz}_q \\ V^{yx}_q & \cdot & \\ V^{zx}_q & & \cdot \end{pmatrix} \begin{pmatrix} y^x_q \\ y^y_q \\ y^z_q \end{pmatrix}$$

3×3 Hermitian Matrix

3 eigenvalues V^1_q, V^2_q, V^3_q

3 eigenvectors

s^1_q, s^2_q, s^3_q

$$H = \sum_{q,\mu} \left[\frac{1}{2M} p_q^{\mu +} p_q^{\mu} + \frac{1}{2} V_q^{\mu} y_q^{\mu +} y_q^{\mu} \right]$$

$$y_q^{\mu} = \vec{y}_q \cdot \vec{S}_q^{\mu} \;, \quad \mu = 1, 2, 3$$

$$H = \sum_{q,\mu} \left[\frac{1}{2M} P_q^{\mu +} P_q^{\mu} + \frac{1}{2} V_q^{\mu} y_q^{\mu +} y_q^{\mu} \right]$$

$\uparrow$ diagonal

$y_q^{\mu} = \vec{y}_q \cdot \vec{S}_q^{\mu}$, $\mu = 1, 2, 3$

$$H = \sum_{q,\mu} \left[\frac{1}{2M} p_q^{\mu +} p_q^{\mu} + \frac{1}{2} V_q^{\mu} y_q^{\mu +} y_q^{\mu} \right]$$

$\uparrow$ diagonal

$$y_q^{\mu} = \vec{y}_q \cdot \vec{S}_q^{\mu} \quad , \quad \mu = 1,2,3$$

Frequencies: $\omega_{q\mu} = \sqrt{\dfrac{V_q^{\mu}}{M}} \quad , \quad \mu = 1,2,3$

$\left. y^{\mu}_{q} y^{\mu +}_{q} y^{\mu}_{q} \right]$

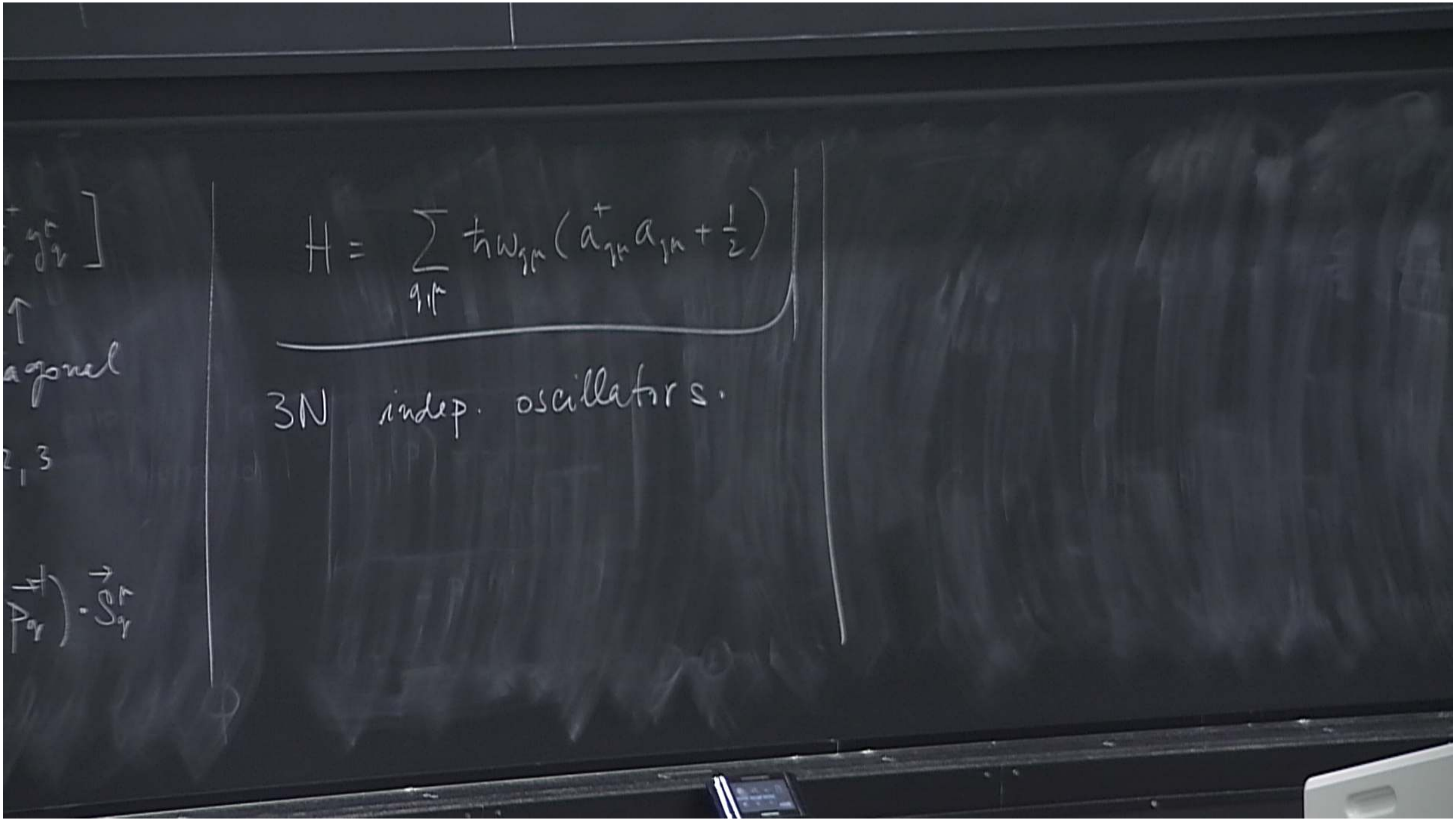
$\uparrow$
diagonal

$= 1, 2, 3$

$\left(\ldots + i \vec{p}_q \right) \cdot \vec{S}^{\mu}_q$

$$H = \sum_{q,\mu} \hbar \omega_{q\mu} \left(a^{+}_{q\mu} a_{q\mu} + \frac{1}{2} \right)$$

3N indep. oscillators.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(bosons)

Phonon specific heat

$$[a_{q\mu}, a^{+}_{q'\mu'}] = \delta_{qq'}\delta_{\mu\mu'}$$

Internal energy of H

Bose Einstein distribution $n_{q\mu}$

$$U(T) = \langle H \rangle_T = \sum_{\vec{q},\mu} \hbar\omega_{q\mu}\left(\langle a^{+}_{q\mu} a_{q\mu}\rangle + \frac{1}{2}\right)$$

$$= \sum_{\vec{q},\mu} \hbar\omega_{q\mu}\left[\frac{1}{e^{\beta\hbar\omega_{q\mu}} - 1} + \frac{1}{2}\right]$$

(bosons)

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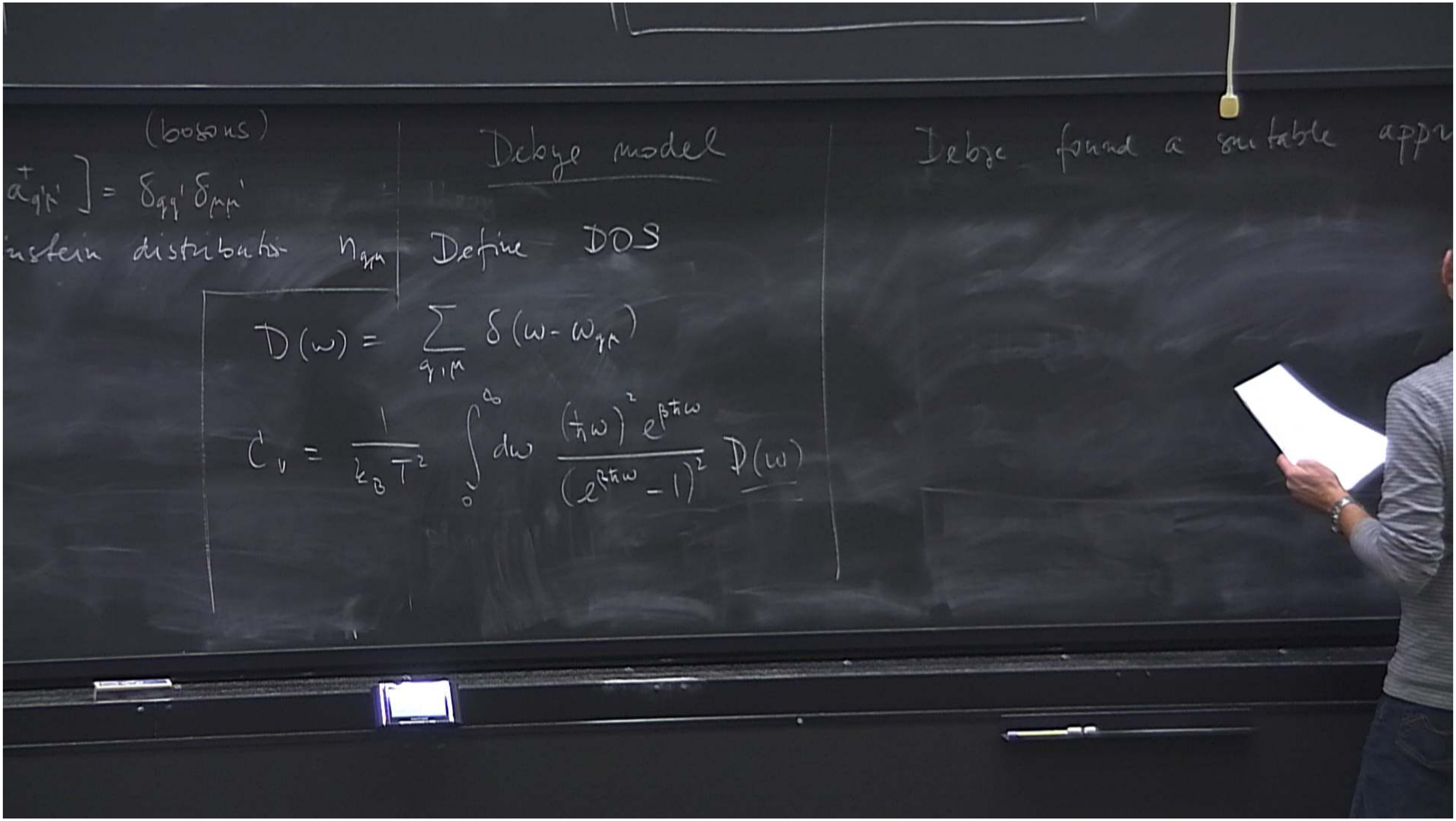
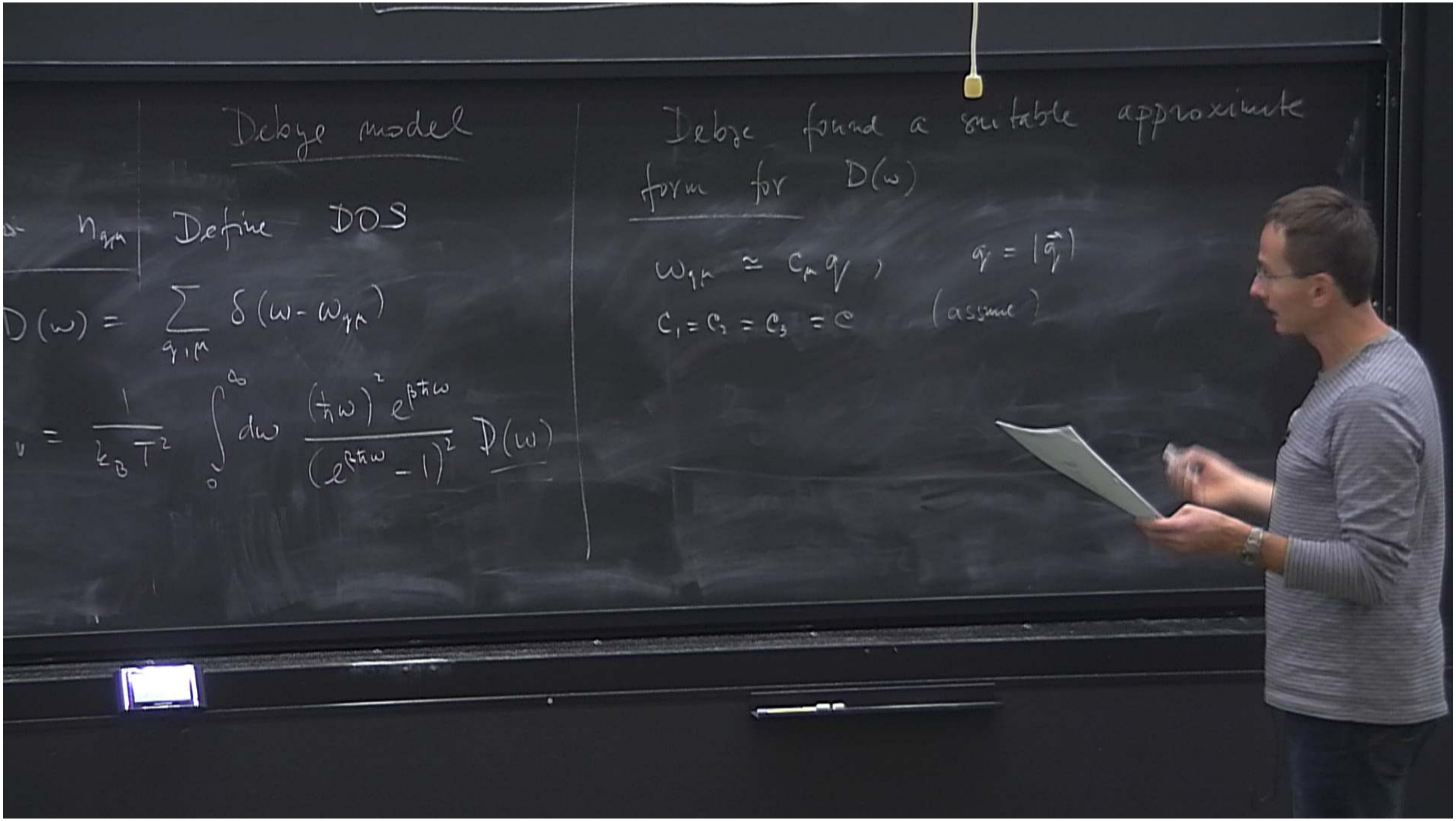
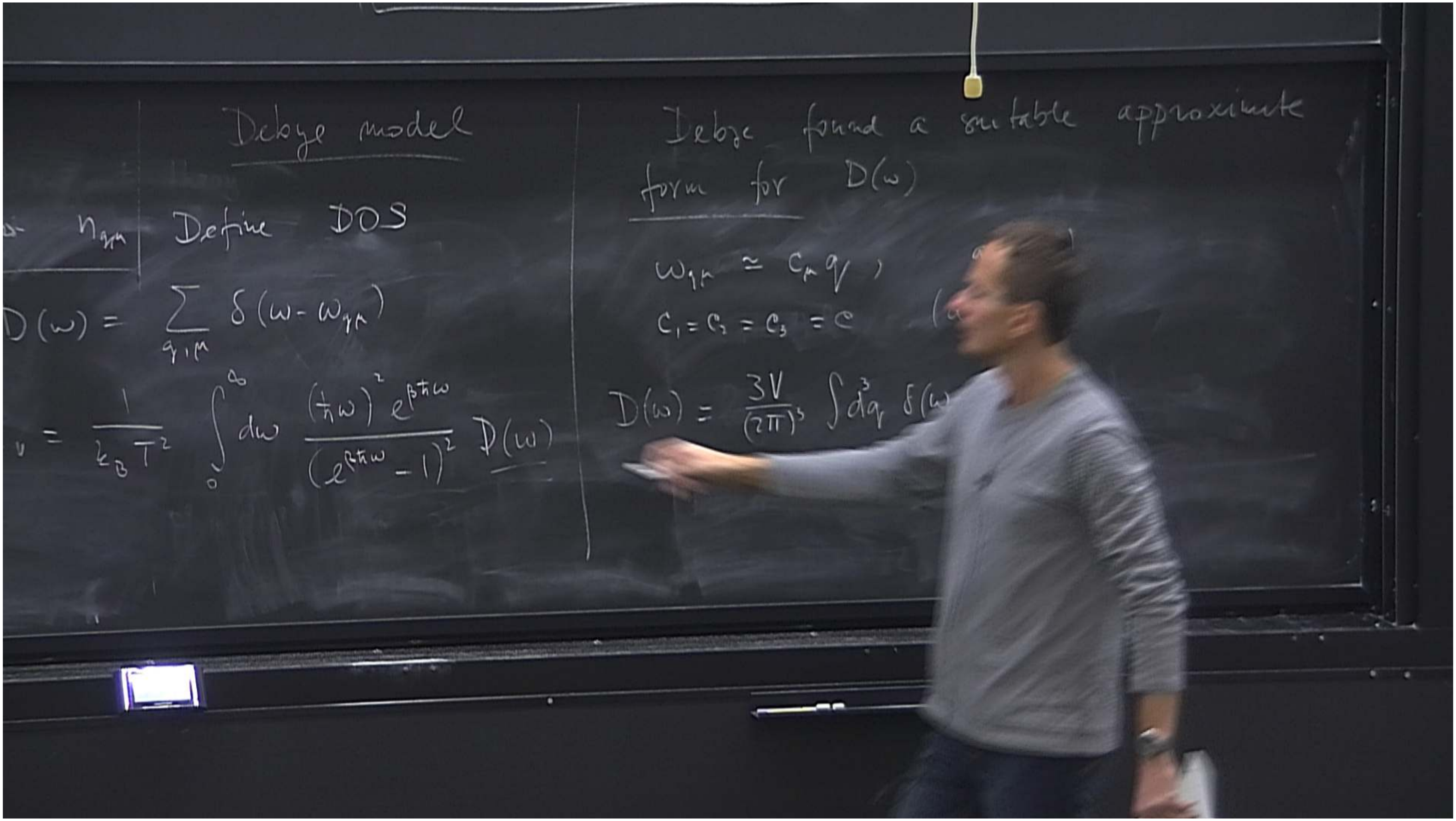
Spec. heat:

$$\boxed{c_V = \frac{dU(T)}{dT} = \frac{1}{k_B T^2}\sum_{q,\mu}\frac{(\hbar\omega_{q\mu})^2 e^{\beta\hbar\omega_{q\mu}}}{[e^{\beta\hbar\omega_{q\mu}} - 1]^2}}$$


(bosons)
$[\ldots a^\dagger_{q'\mu'}] = \delta_{qq'}\delta_{\mu\mu'}$
...instein distribution $n_{q\mu}$
Debye model
Define DOS
$D(\omega) = \sum_{q,\mu} \delta(\omega - \omega_{q\mu})$
$C_V = \frac{1}{k_B T^2} \int_0^\infty d\omega \, \frac{(\hbar\omega)^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2} D(\omega)$
Debye found a suitable appr...


Debye model
$n_{q\mu}$
Define DOS
$D(\omega) = \sum_{q,\mu} \delta(\omega - \omega_{q\mu})$
$= \frac{1}{k_B T^2} \int_0^\infty d\omega \frac{(\hbar\omega)^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2} D(\omega)$
Debye found a suitable approximate form for $D(\omega)$
$\omega_{q\mu} \simeq c_\mu q$, $q = |\vec{q}|$
$c_1 = c_2 = c_3 = c$ (assume)


Debye model
Define DOS
D(ω) = Σ_{q,μ} δ(ω - ω_{qμ})
= 1/(k_B T^2) ∫_0^∞ dω (ħω)^2 e^{βħω} / (e^{βħω} - 1)^2 D(ω)
Debye found a suitable approximate form for D(ω)
ω_{qμ} ≃ c_μ q ,
c_1 = c_2 = c_3 = c
D(ω) = 3V/(2π)^3 ∫ d^3q δ(ω

Debye model

$n_{q\mu}$ Define DOS

$$D(\omega) = \sum_{q,\mu} \delta(\omega - \omega_{q\mu})$$

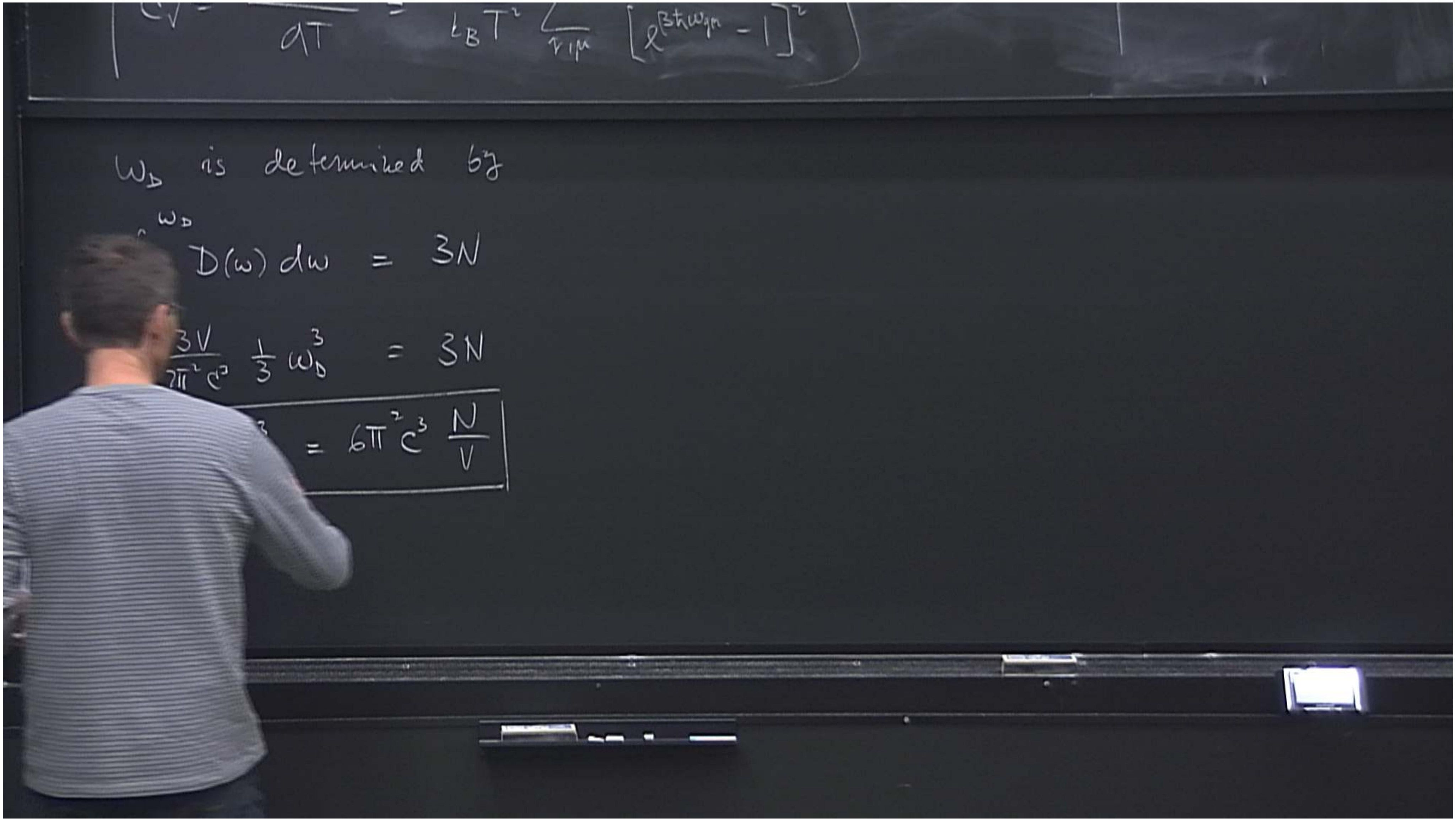
$$_v = \frac{1}{k_B T^2} \int_0^\infty d\omega \frac{(\hbar\omega)^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2} D(\omega)$$

Debye found a suitable approximate form for $D(\omega)$

$\omega_{q\mu} \simeq c_\mu q$, $q = |\vec{q}|$

$c_1 = c_2 = c_3 = c$ (assume)

$$D(\omega) = \frac{3V}{(2\pi)^3} \int d^3q \, \delta(\omega - cq) = \frac{3V}{2\pi^2} \frac{\omega^2}{c^3}$$


ω_D is determined by
D(ω) dω = 3N
3V/2π²c³ · 1/3 ω_D³ = 3N
= 6π² c³ N/V

by

3N

3N

$\boxed{\frac{N}{V}}$

Debye momentum : $k_D = \frac{\omega_D}{c} = \left(6\pi^2 \frac{N}{V}\right)^{1/3} \sim \frac{4}{a}$

Debye temperature $k_B \theta_D = \hbar \omega_D$

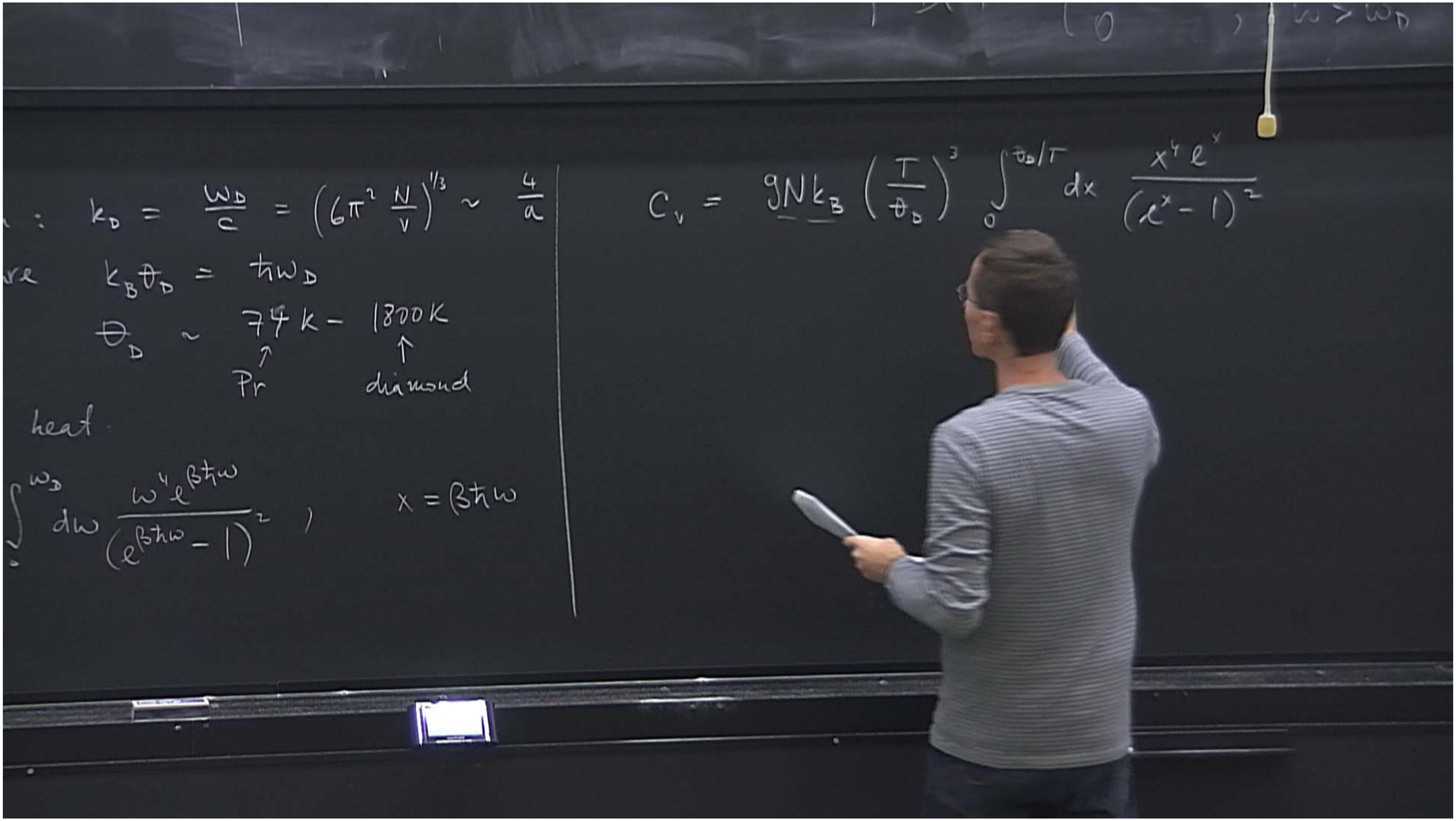
$\theta_D \sim 74\,K - 1800\,K$

Pr diamond

- Back to spec. heat

$$C_V = \frac{3V\hbar^2}{2\pi^2 c^3 k_B T^2} \int_0^{\omega_D} d\omega \frac{\omega^4 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}, \qquad x = \beta\hbar\omega$$

$$C_V = 9Nk_B \left(\frac{T}{\theta_D}\right)^3$$



$\omega > \omega_D$
$k_D = \frac{\omega_D}{c} = \left(6\pi^2 \frac{N}{V}\right)^{1/3} \sim \frac{4}{a}$
$k_B \theta_D = \hbar\omega_D$
$\theta_D \sim 74K - 1800K$
Pr
diamond
heat
$\int^{\omega_D} d\omega \frac{\omega^4 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}$
$x = \beta\hbar\omega$
$C_V = 9Nk_B \left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} dx \frac{x^4 e^x}{(e^x-1)^2}$

$\omega > \omega_D$

$\left(\frac{N}{V}\right)^{1/3} \sim \frac{4}{a}$

1800 K

$\uparrow$

diamond

$x = \beta\hbar\omega$

$$C_V = 9Nk_B\left(\frac{T}{\theta_D}\right)^3 \underbrace{\int_0^{\theta_D/T} dx \, \frac{x^4 e^x}{(e^x-1)^2}}_{f_D\left(\frac{\theta_D}{T}\right)}$$

• Low T $\quad (T \ll \theta_D) \quad x_D \equiv \frac{\theta_D}{T} \gg 1$

$$f(x_D) \simeq \underbrace{\int_0^\infty dx \, \frac{x^4 e^x}{(e^x-1)^2}}_{\frac{4\pi^4}{15}} - \underbrace{\int_{x_D}^\infty dx \cdots}_{\sim e^{-x_D} \ll 1}$$

$$C_V \simeq \frac{12\pi^4}{5} N k_B \left(\frac{T}{\theta_D}\right)^3$$

$$T \ll \theta_D$$

• High T $(T \gg \theta_D)$ $x_D \ll 1$

expand $e^x \simeq 1 + x \ldots$

$$f(x_D) \simeq \int_0^{x_D} dx \frac{x^4}{(1+x-1)^2} = \int_0^{x_D} dx\, x^2 = \frac{1}{3} x_D^3$$

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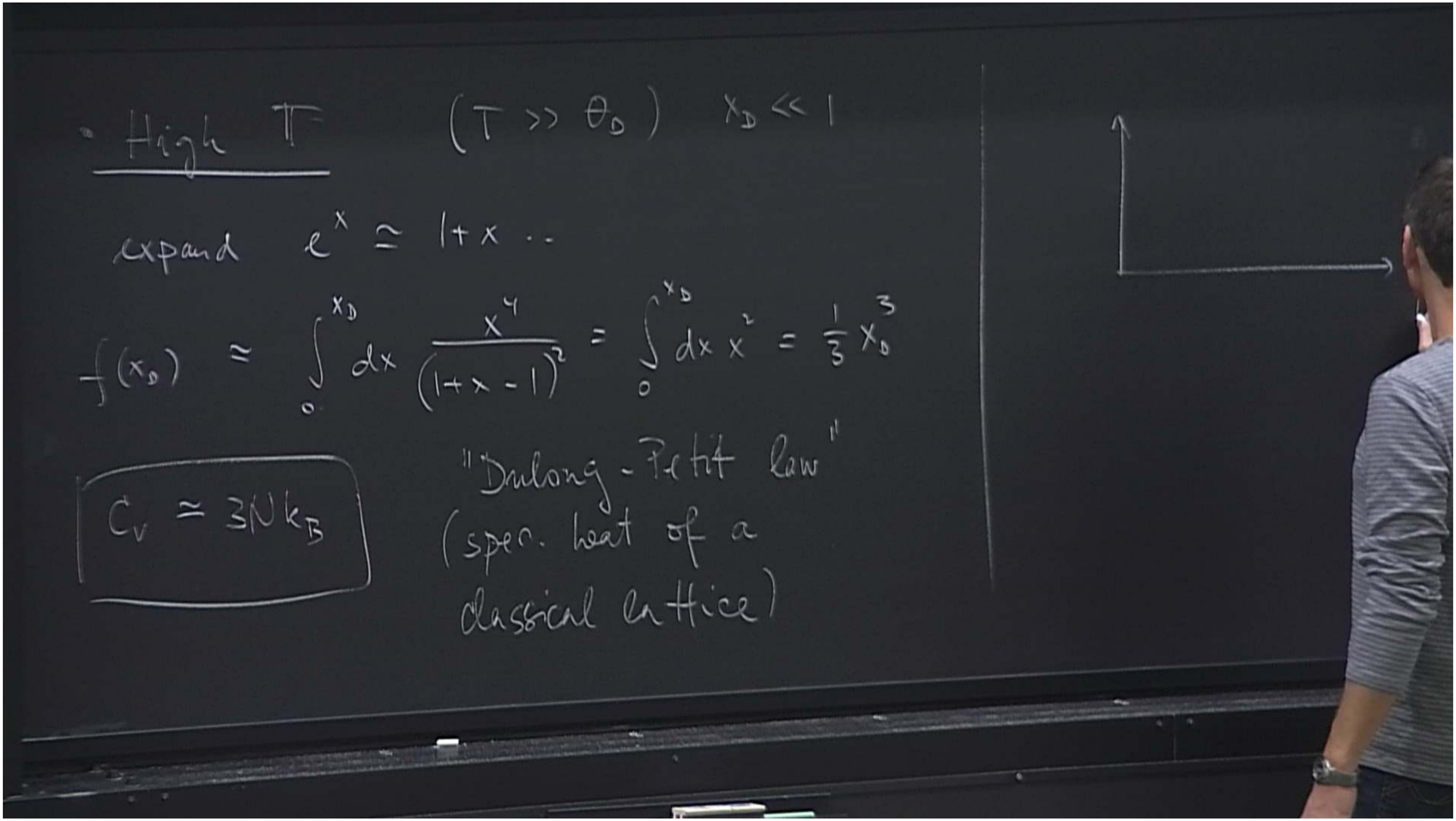
$$\boxed{C_V \simeq 3Nk_B}$$

"Dulong - Petit law"
(spec. heat of a
classical lattice)



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T $\quad (T \gg \theta_D) \quad x_D \ll 1$

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$$\simeq \int_0^{x_D} dx \, \frac{x^4}{(1+x-1)^2} = \int_0^{x_D} dx \, x^2 = \frac{1}{3} x_D^3$$

$\boxed{3Nk_B}$

"Dulong-Petit law"
(spec. heat of a classical lattice)