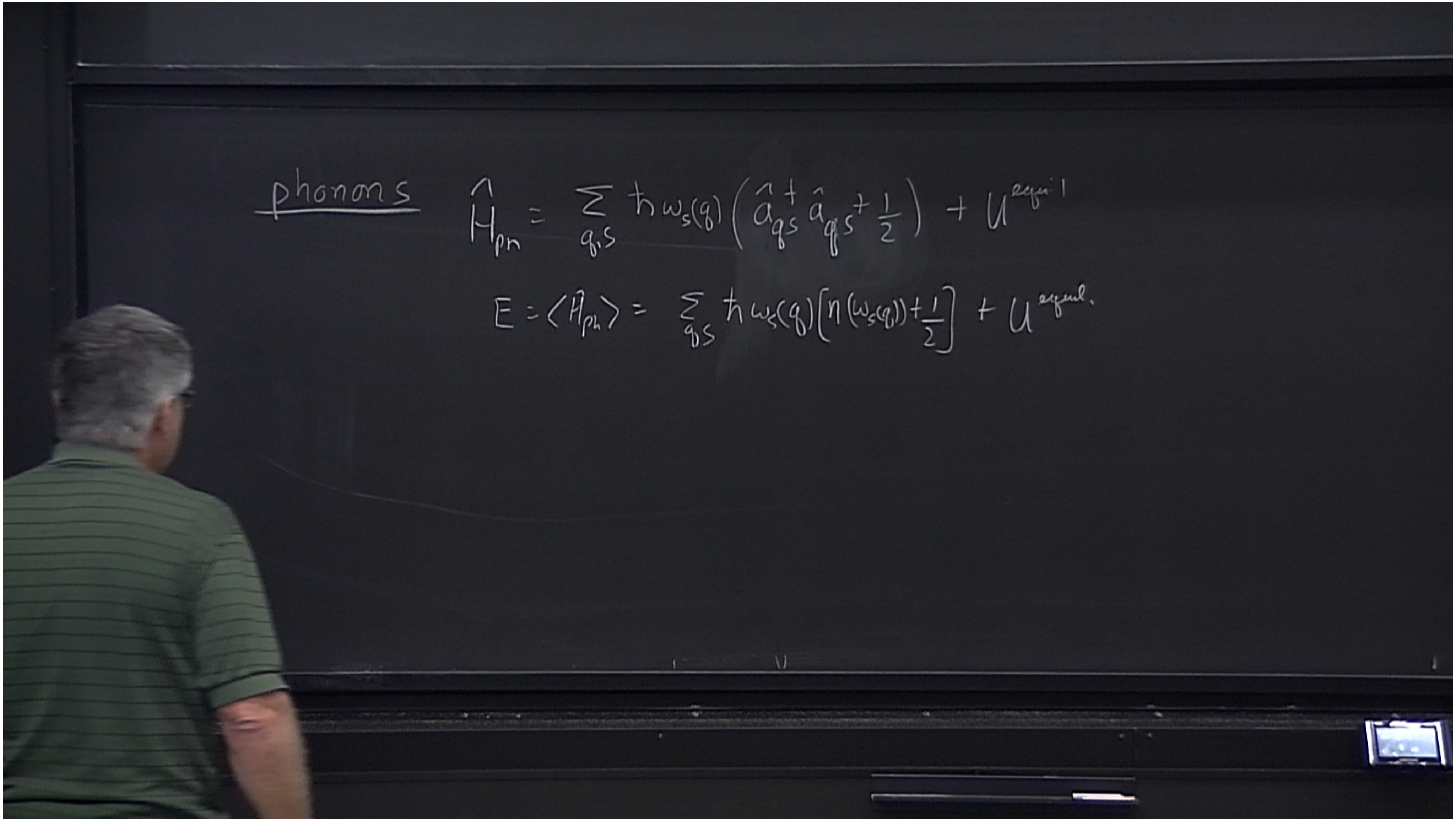
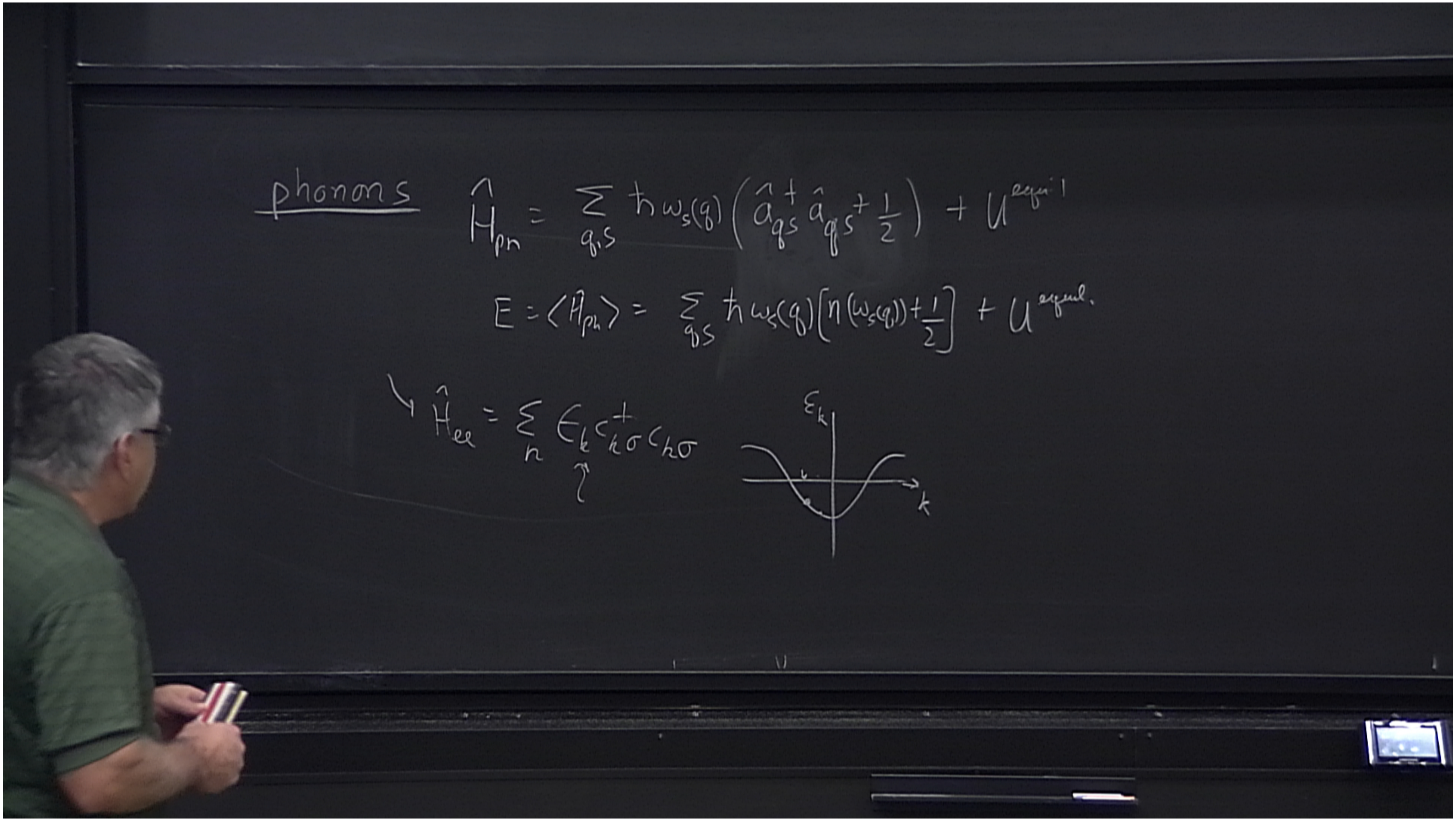
Title: PSI 2016/2017 Condensed Matter - Lecture 7

Date: Nov 15, 2016 10:45 AM

URL: http://pirsa.org/16110058

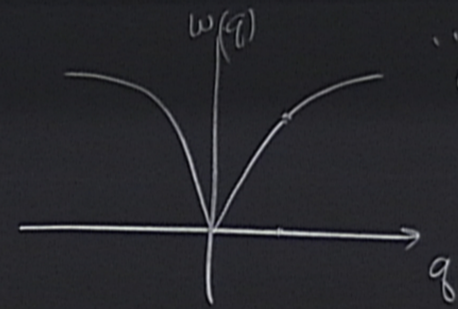
Abstract:


phonons
$\hat{H}_{ph} = \sum_{q,s} \hbar \omega_s(q) \left(\hat{a}^{\dagger}_{qs} \hat{a}_{qs} + \frac{1}{2} \right) + U^{equil}$
$E = \langle \hat{H}_{ph} \rangle = \sum_{qs} \hbar \omega_s(q) \left[n(\omega_s(q)) + \frac{1}{2} \right] + U^{equil.}$


phonons
$\hat{H}_{ph} = \sum_{q,s} \hbar\omega_s(q)\left(\hat{a}^\dagger_{qs}\hat{a}_{qs} + \frac{1}{2}\right) + U^{equil}$
$E = \langle \hat{H}_{ph} \rangle = \sum_{qs} \hbar\omega_s(q)\left[n(\omega_s(q)) + \frac{1}{2}\right] + U^{equil.}$
$\hat{H}_{ee} = \sum_{k} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma}$
?
ε_k
k

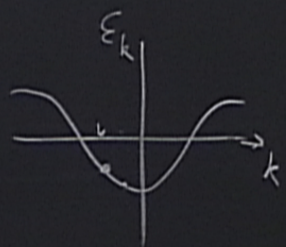
$$\hat{H}_{ph} = \sum_{q,s} \hbar\,\omega_s(q)\left(\hat{a}^{\dagger}_{qs}\hat{a}_{qs} + \frac{1}{2}\right) + U^{equil}$$

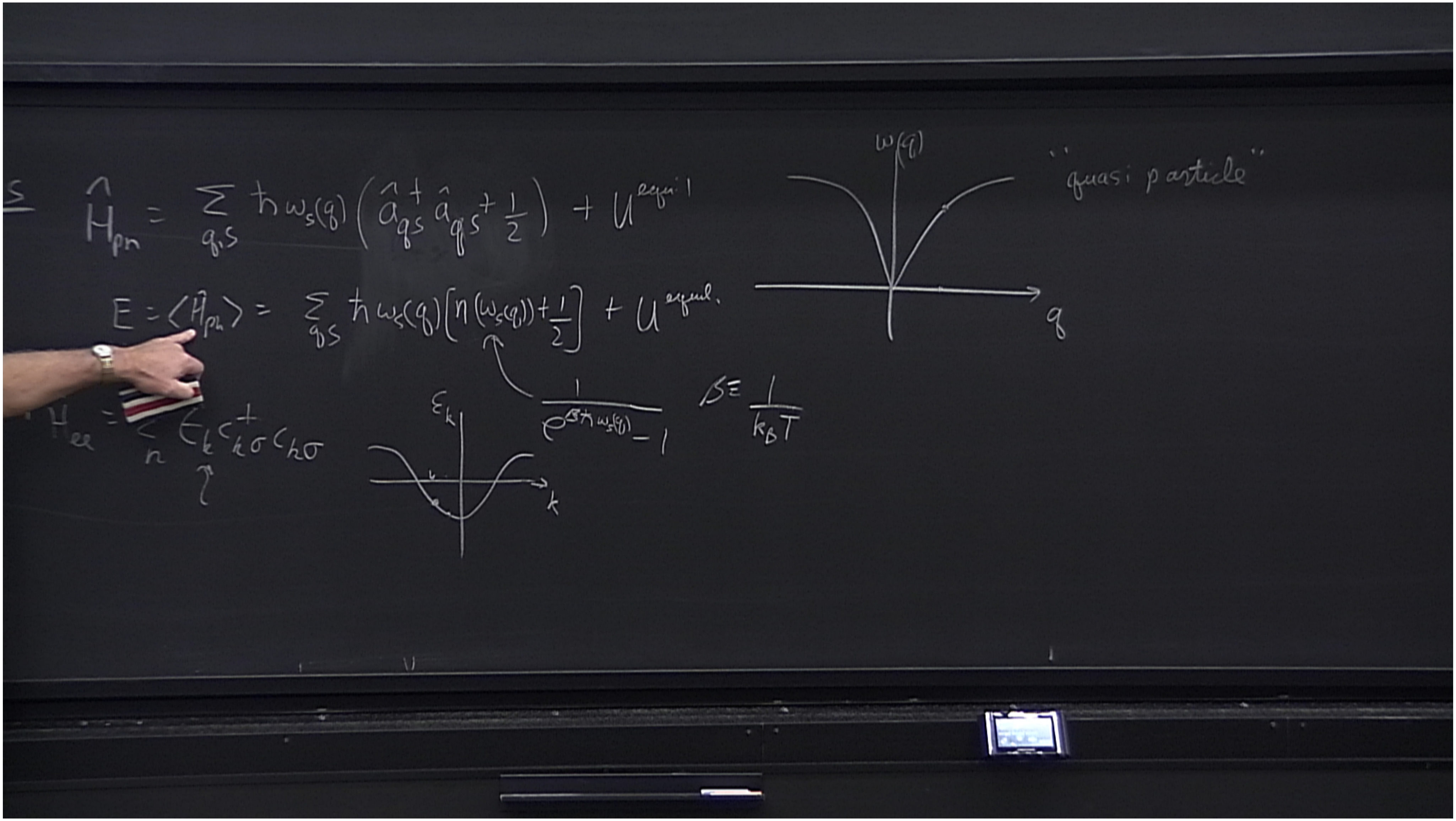
$$E = \langle \hat{H}_{ph} \rangle = \sum_{qs} \hbar\,\omega_s(q)\left[n(\omega_s(q)) + \frac{1}{2}\right] + U^{equil.}$$



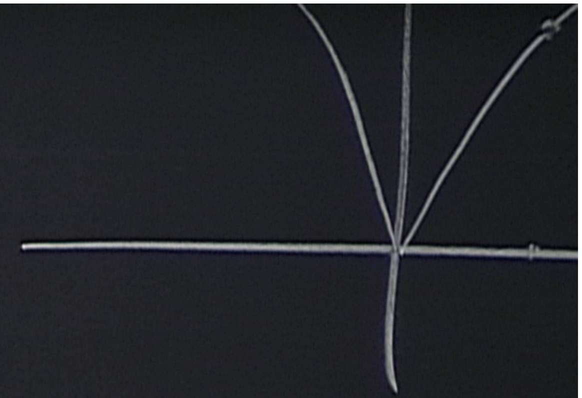
"quasi particle"

$$\hat{H}_{el} = \sum_{k} \epsilon_k\, c^{\dagger}_{k\sigma} c_{k\sigma}$$




$\hat{H}_{ph} = \sum_{q,s} \hbar\omega_s(q)\left(\hat{a}^{\dagger}_{qs}\hat{a}_{qs} + \frac{1}{2}\right) + U^{equil}$
$E = \langle \hat{H}_{ph} \rangle = \sum_{qs} \hbar\omega_s(q)\left[n(\omega_s(q)) + \frac{1}{2}\right] + U^{equil.}$
$\frac{1}{e^{\beta\hbar\omega_s(q)} - 1}$
$\beta \equiv \frac{1}{k_B T}$
$H_{ee} = \sum_k \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma}$
ϵ_k
k
$\omega(q)$
q
"quasi particle"

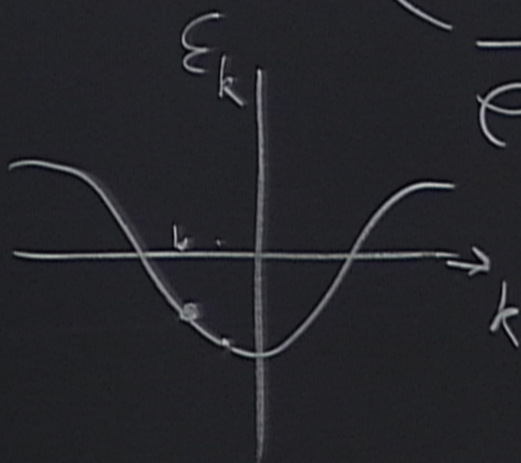
$$\sum_{q,s} \hbar\omega_s(q)\left(a^\dagger_{qs}a_{qs}+\frac{1}{2}\right)+U$$

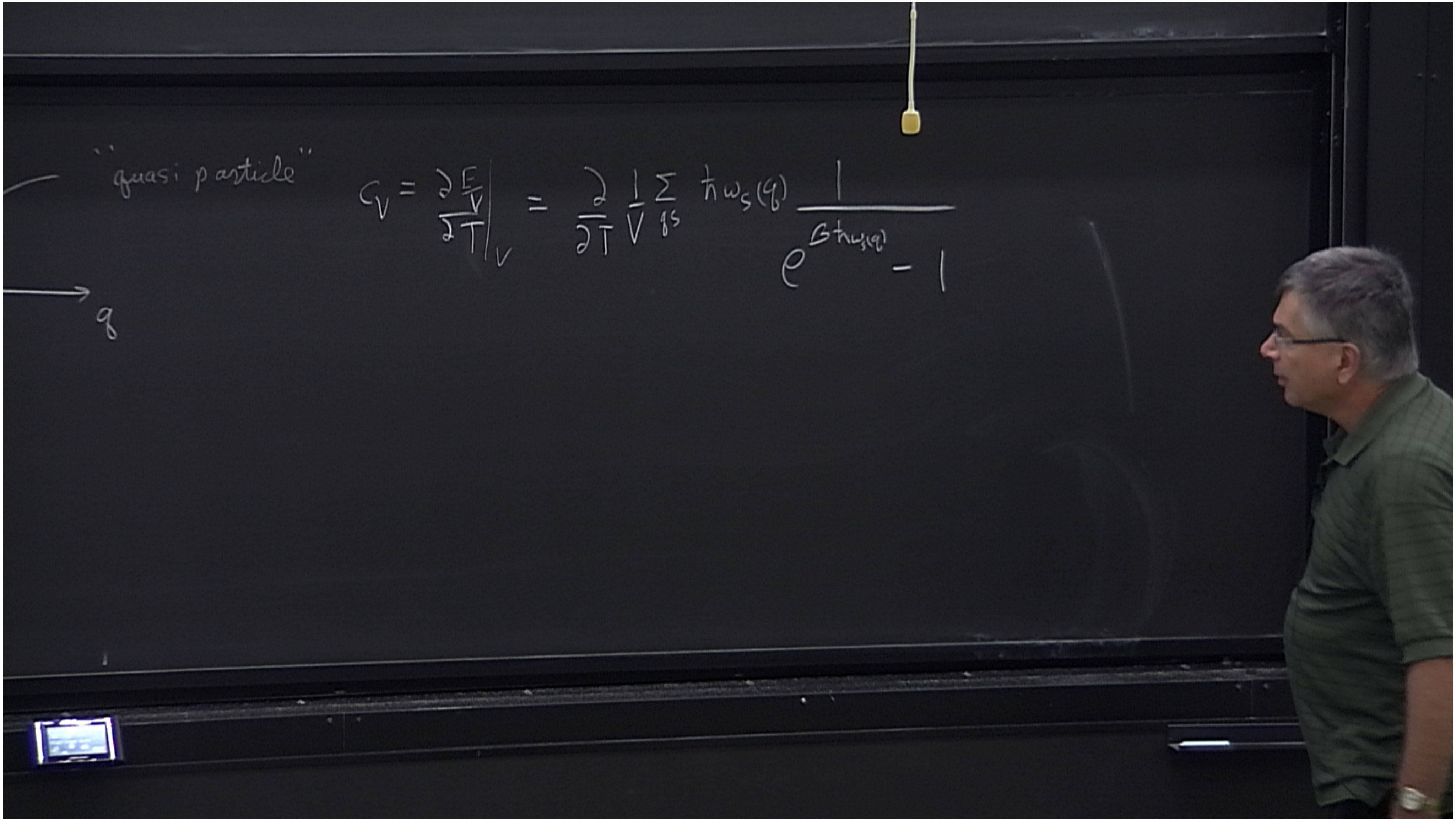


$$\langle \ldots_{ph}\rangle = \sum_{qs}\hbar\omega_s(q)\left[n(\omega_s(q))+\frac{1}{2}\right]+U^{\text{equil.}}$$

$$n(\omega_s(q)) = \frac{1}{e^{\beta\hbar\omega_s(q)}-1} \qquad \beta \equiv \frac{1}{k_B T}$$

$$c^\dagger_{k\sigma}c_{k\sigma}$$




"quasi particle"
$c_V = \frac{\partial \frac{E}{V}}{\partial T}\Big|_V = \frac{\partial}{\partial T}\frac{1}{V}\sum_{qs} \hbar\omega_s(q)\frac{1}{e^{\beta\hbar\omega_s(q)}-1}$
q

particle"

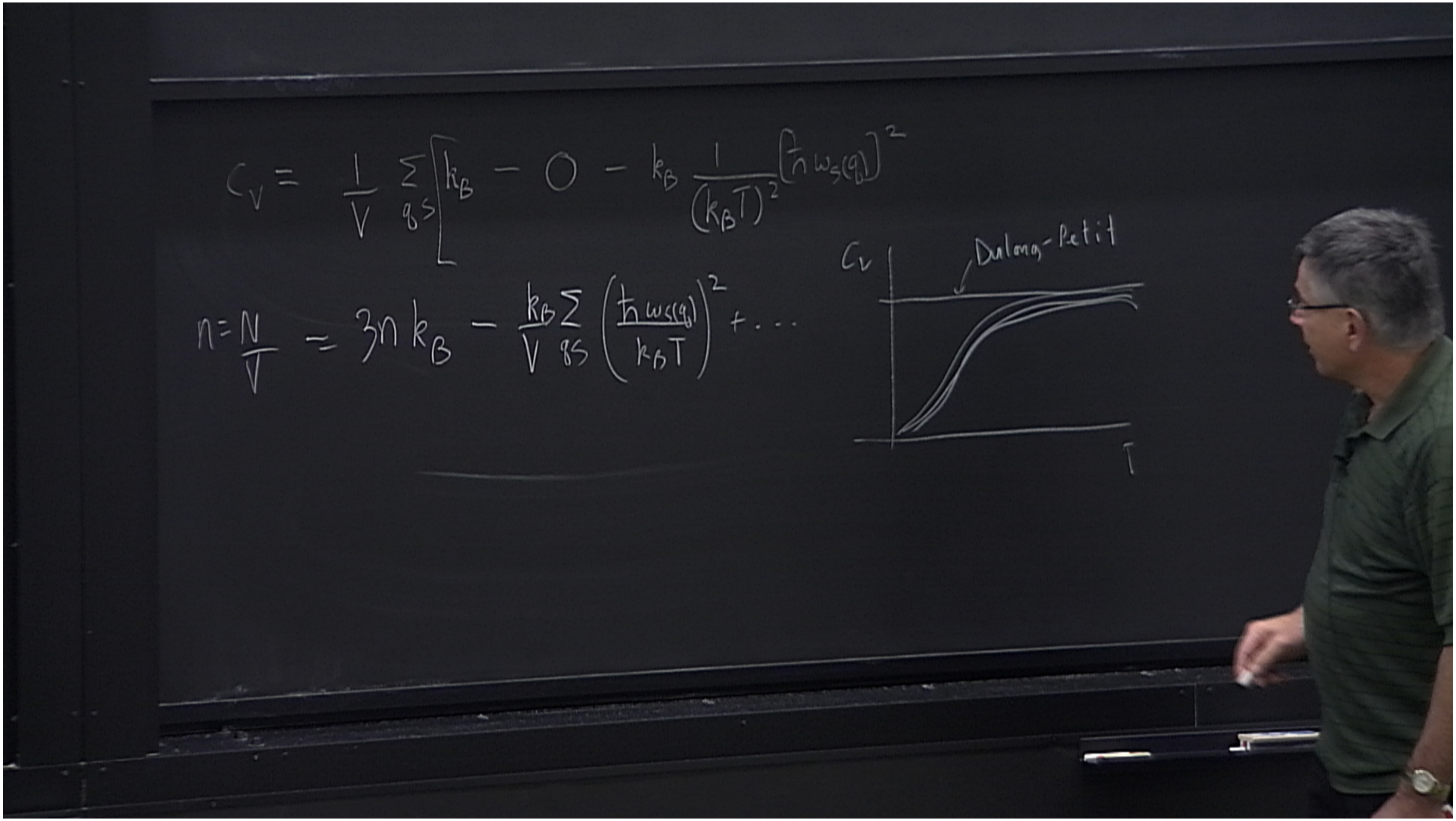
$$C_V = \frac{\partial \frac{E}{V}}{\partial T}\Big|_V = \frac{\partial}{\partial T} \frac{1}{V} \sum_{qs} \hbar \omega_s(q) \frac{1}{e^{\beta \hbar \omega_s(q)} - 1}$$

1) high temperature $(\beta \to 0)$

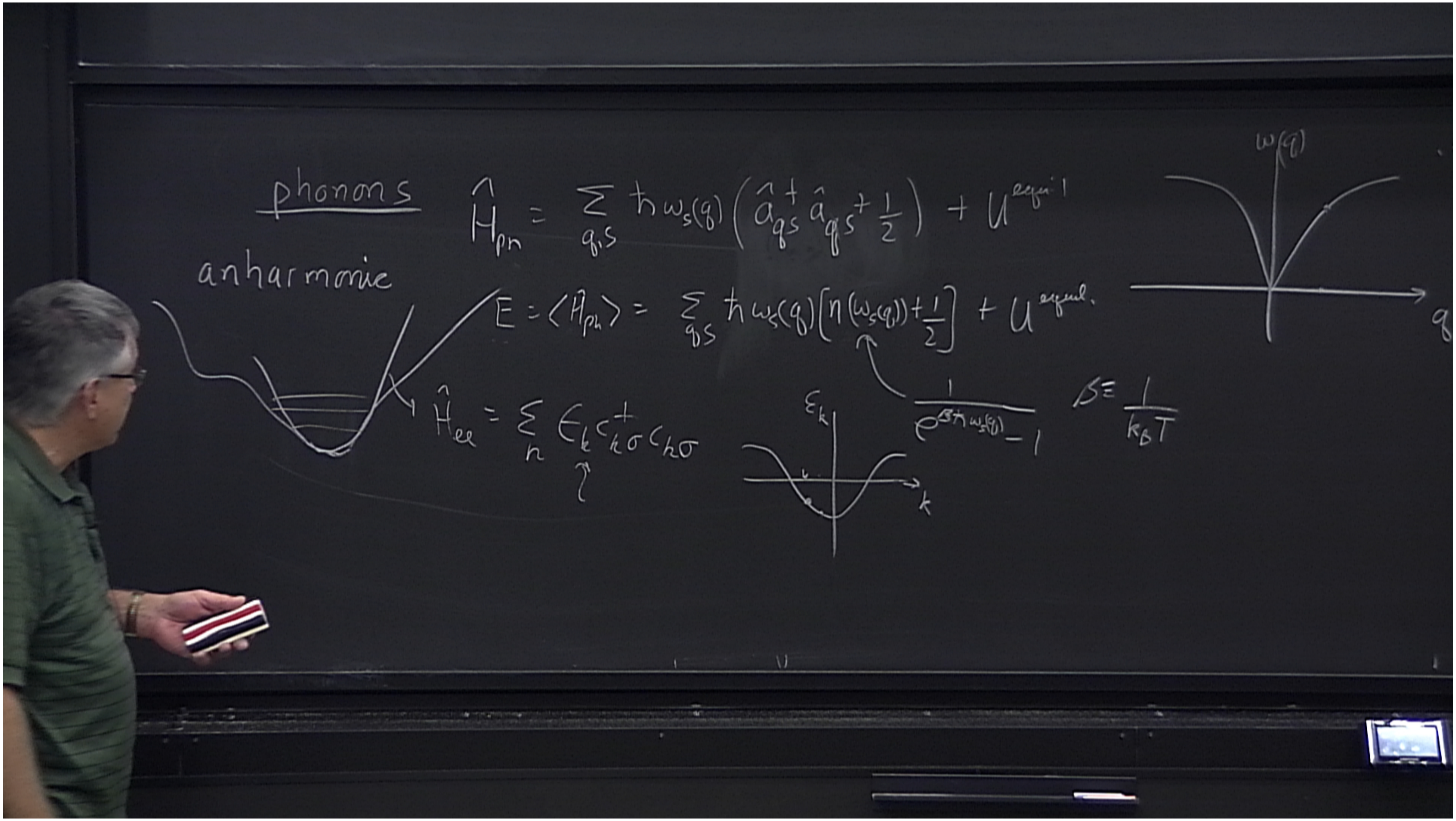
$$\frac{1}{e^x - 1} \sim \frac{1}{x}\left(1 - \frac{x}{2} + \frac{x^2}{12}\right)$$

for $T \to \infty$

$$C_V = \frac{\partial}{\partial T} \frac{1}{V} \sum_{qs} \frac{\hbar \omega_s(q)}{\beta \hbar \omega_s(q)} \left(1 - \frac{\beta \hbar \omega_s(q)}{2} + \frac{\left[\beta \hbar \omega_s(q)\right]^2}{12} + \dots\right)$$



$C_V = \frac{1}{V}\sum_{qs}\Big[k_B - 0 - k_B\frac{1}{(k_BT)^2}\big[\hbar\omega_s(q)\big]^2$
$n = \frac{N}{V}$
$\simeq 3n\,k_B - \frac{k_B}{V}\sum_{qs}\left(\frac{\hbar\omega_s(q)}{k_BT}\right)^2 + \ldots$
C_V
Dulong-Petit
T

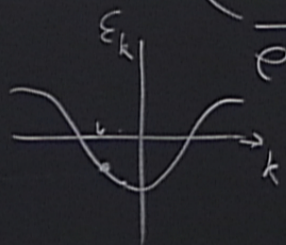

phonons
$\hat{H}_{ph} = \sum_{q,s} \hbar\omega_s(q)\left(\hat{a}^\dagger_{qs}\hat{a}_{qs}+\frac{1}{2}\right) + U^{equil}$
anharmonic
$E = \langle \hat{H}_{ph}\rangle = \sum_{qs}\hbar\omega_s(q)\left[n(\omega_s(q))+\frac{1}{2}\right] + U^{equil.}$
$\frac{1}{e^{\beta\hbar\omega_s(q)}-1}$
$\beta \equiv \frac{1}{k_B T}$
$\hat{H}_{el} = \sum_{k} \epsilon_k c^\dagger_{k\sigma}c_{k\sigma}$
ϵ_k
k
$\omega(q)$
q

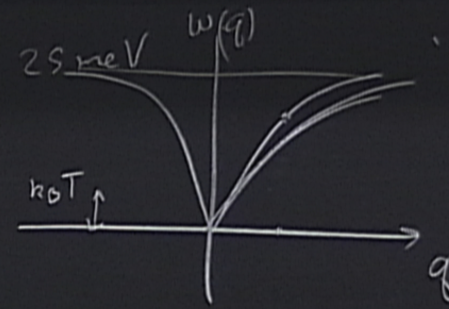
$$\hat{H}_{ph} = \sum_{q,s} \hbar\omega_s(q)\left(\hat{a}^\dagger_{qs}\hat{a}_{qs} + \frac{1}{2}\right) + U^{equil}$$

$$E = \langle \hat{H}_{ph} \rangle = \sum_{qs} \hbar\omega_s(q)\left[n(\omega_s(q)) + \frac{1}{2}\right] + U^{equil.}$$

$$n(\omega_s(q)) = \frac{1}{e^{\beta\hbar\omega_s(q)} - 1} \qquad \beta \equiv \frac{1}{k_B T}$$

$$\hat{H}_{el} = \sum_{k} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma}$$



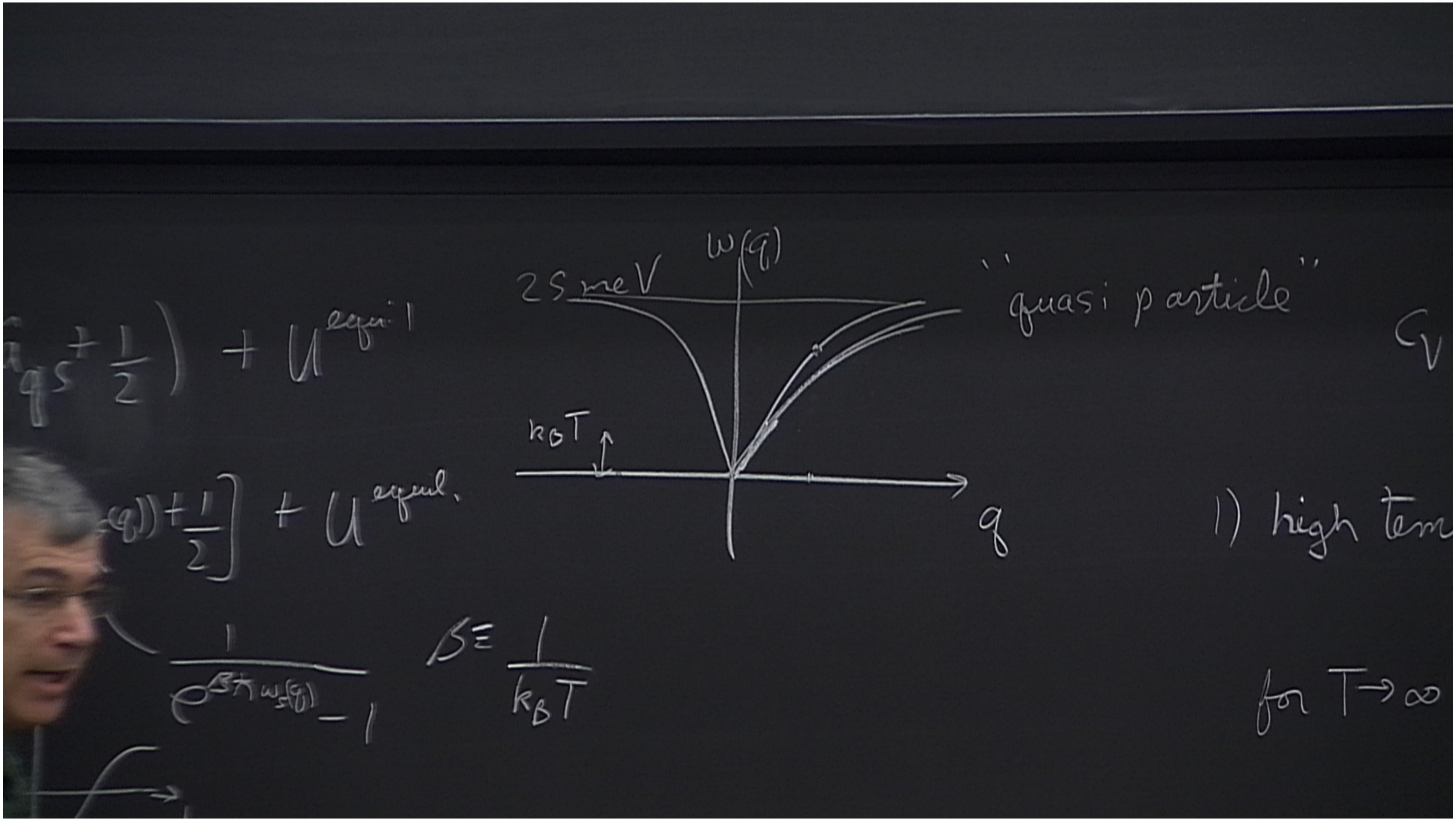


"quasi particle"

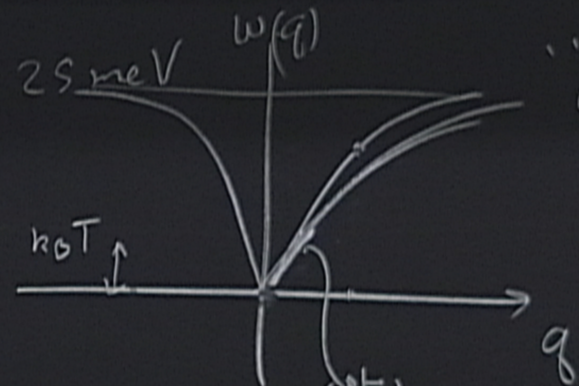
$$C_V = \frac{\partial E}{\partial T}\bigg|_V$$

1) high temperature

for $T \to \infty$ $C_V = \frac{\partial}{\partial}$


$q s + \frac{1}{2}) + U^{equil}$
$(q)) + \frac{1}{2}] + U^{equil.}$
$\frac{1}{e^{\beta\hbar\omega_s(q)} - 1}$
$\beta \equiv \frac{1}{k_B T}$
$\omega(q)$
25 meV
"quasi particle"
$k_B T$
q
C_V
1) high tem
for $T \to \infty$

$\omega_s(q)\left(\hat{a}^{\dagger}_{qs}\hat{a}_{qs}+\frac{1}{2}\right)+U^{\text{equil}}$



"quasi particle"

$C_V=\frac{\partial E}{\partial T}$

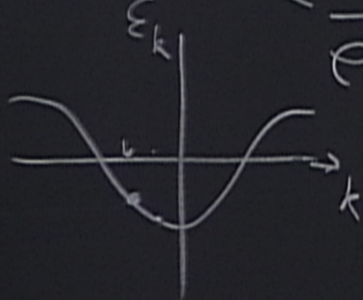
$\sum_{qs}\hbar\omega_s(q)\left[n(\omega_s(q))+\frac{1}{2}\right]+U^{\text{equil.}}$

$\frac{1}{e^{\beta\hbar\omega_s(q)}-1}$ $\qquad \beta\equiv\frac{1}{k_B T}$

$\omega_s(q)\sim c_s(\hat{k})|k|$ $\qquad \lambda\sim\frac{2\pi}{q}$

1) high temperature

for $T\to\infty$ $\quad C_V=$

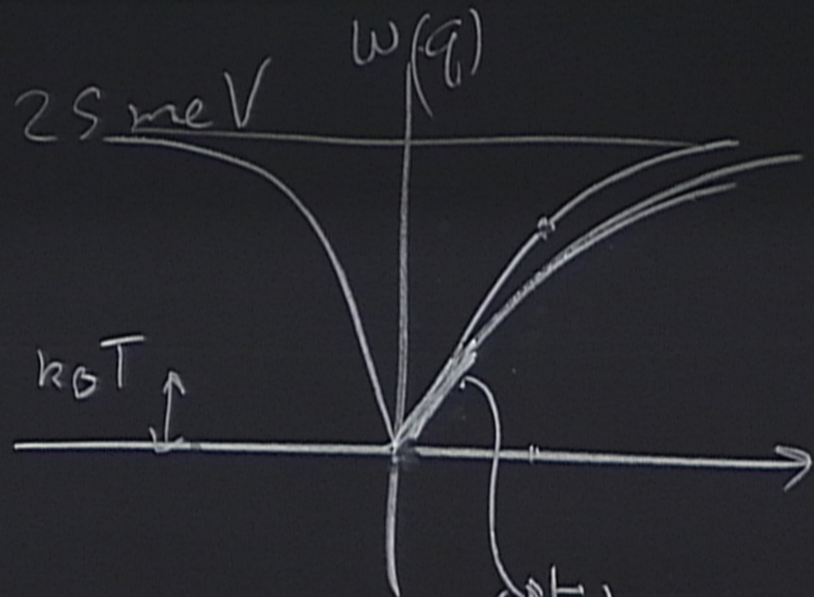


$$) + U^{\text{equil}}$$

$$(q)) + \frac{1}{2}\Big] + U^{\text{equil.}}$$

$$\frac{1}{e^{\beta\hbar\omega_s(q)} - 1}$$

$$\beta \equiv \frac{1}{k_B T}$$



''quasi particl

$$\omega_s(q) \sim c_s |\vec{k}|\,|k| \qquad \lambda \sim \frac{2\pi}{q}$$

k

2) Low temperature

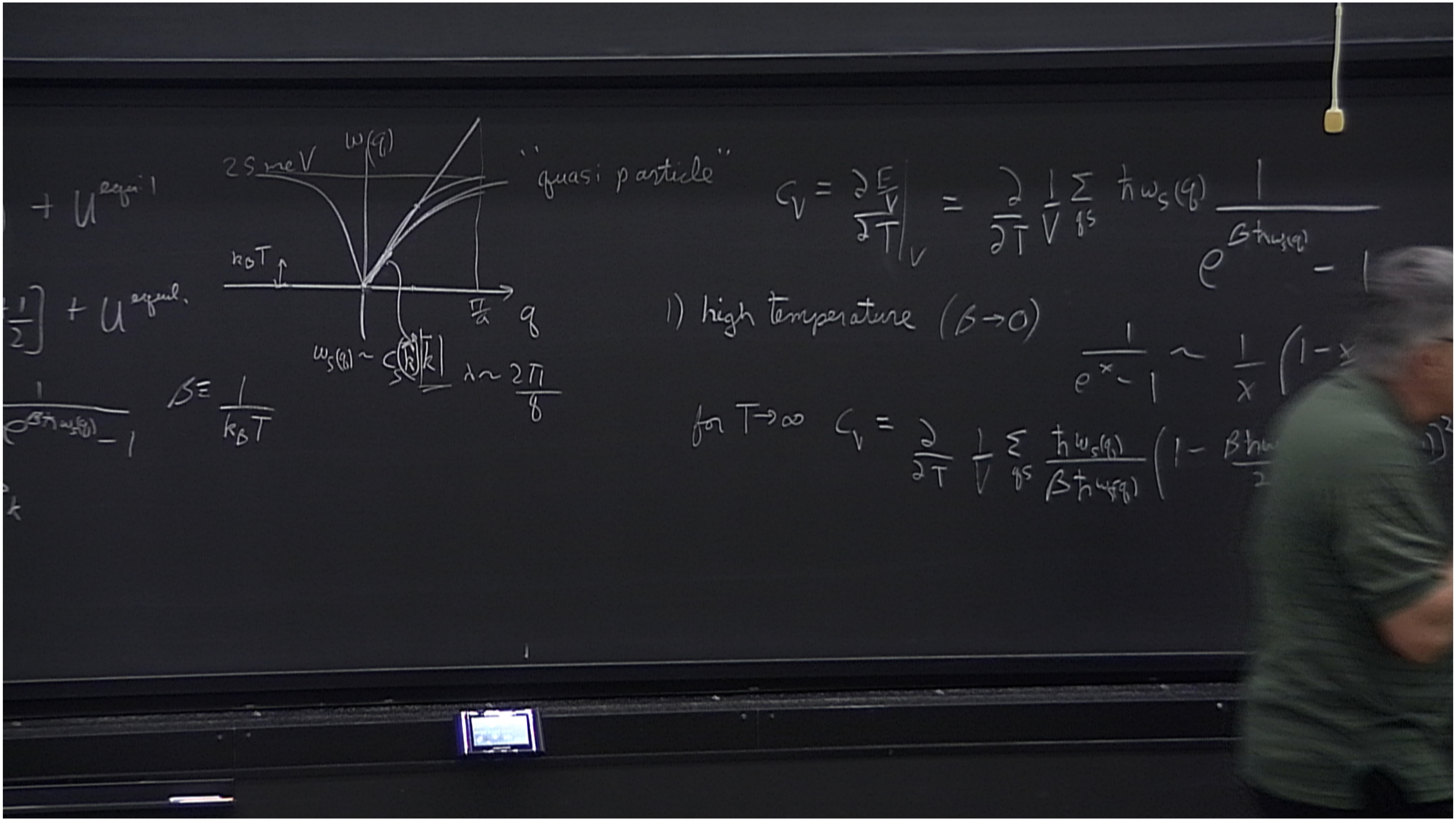
$$c_V \sim \frac{\partial}{\partial T}\left(\frac{1}{V}\sum_{q,s} \frac{\hbar c_s(\hat{q})\, q}{e^{\beta \hbar c_s(\hat{q})\, q} - 1}\right)$$

$$\int \frac{d^3q}{(2\pi)^3} \rightarrow \int_{\text{all angles}} \frac{d\Omega}{4\pi} \int_0 \frac{dk}{2\pi^2}$$

2) Low temperature

$$c_V \sim \frac{\partial}{\partial T}\left(\frac{1}{V}\sum_{\vec{q}, s} \frac{\hbar c_s(\hat{q})\, q}{e^{\beta \hbar c_s(\hat{q})\, q}-1}\right)$$

$$\int \frac{d^3q}{(2\pi)^3} \to \int_{\text{all angles}} \frac{d\Omega}{4\pi} \int_0 \frac{dq\, q^2}{2\pi^2}$$



ω(q)
25 meV
"quasi particle"
$k_B T$
π/a
q
$\omega_s(q) \sim c_s |k|$
$\lambda \sim 2\pi/q$
$\beta \equiv \frac{1}{k_B T}$
$C_V = \frac{\partial E/V}{\partial T}\Big|_V = \frac{\partial}{\partial T}\frac{1}{V}\sum_{qs}\hbar\omega_s(q)\frac{1}{e^{\beta\hbar\omega_s(q)}-1}$
1) high temperature (β→0)
for T→∞

$x = \beta \hbar c_s(\hat{q})\, q$

2) Low temperature

$$C_V \sim \frac{\partial}{\partial T}\left(\frac{1}{V}\sum_{q,s}\right) \frac{\hbar c_s(\hat{q})\, q}{e^{\beta\hbar c_s(\hat{q}) q} - 1} = \frac{\partial}{\partial T} \sum_s \int \frac{d\Omega}{4\pi} \int_0^\infty \frac{dx}{2\pi^2} \frac{x^3\, \hbar c_s(\hat{q})}{[\beta \hbar c_s(\hat{q})]^4}$$

$$\int \frac{d^3q}{(2\pi)^3} \to \int_{\text{all angles}} \frac{d\Omega}{4\pi} \int_0^\infty \frac{dq}{2\pi^2}\, q^2$$

-Petit

T

$x = \beta \hbar c_s(\hat{q})\, q$

2) low temperature

$$c_V \sim \frac{\partial}{\partial T}\left(\frac{1}{V}\sum_{q,s}\right)\frac{\hbar c_s(\hat{q})\, q}{e^{\beta\hbar c_s(\hat{q}) q} - 1} = \frac{\partial}{\partial T}\sum_s \int\frac{d\Omega}{4\pi}\int_0^\infty \frac{dx}{2\pi^2}\frac{x^3\, \hbar c_s(\hat{q})}{[\beta\hbar c_s(\hat{q})]^4}\frac{1}{e^x - 1}$$

$$\int\frac{d^3q}{(2\pi)^3} \to \int_{\text{all angles}}\frac{d\Omega}{4\pi}\int_0^\infty\frac{dq}{2\pi^2}\, q^2$$

-Petit

T

$$x = \beta \hbar c_s(\hat{q})\, q$$

$$\frac{1}{3}\sum_s \int \frac{d\Omega}{4\pi} \frac{1}{(c_s(\hat{q}))^3} \equiv \frac{1}{c^2}$$

$$\frac{\hbar c_s(\hat{q})\, q}{e^{\beta \hbar c_s(\hat{q}) q} - 1} = \frac{\partial}{\partial T} \sum_s \int \frac{d\Omega}{4\pi} \int_0^\infty \frac{dx}{2\pi^2} \frac{x^3 \hbar c_s(\hat{q})}{[\beta \hbar c_s(\hat{q})]^4} \frac{1}{e^x - 1}$$

$$\int_{\text{all angles}} \frac{d\Omega}{4\pi} \int_0^\infty \frac{dq}{2\pi^2}\, q^2$$

$x = \beta \hbar c_s(\hat{q})\, q$

$$\frac{1}{3}\sum_s \int \frac{d\Omega}{4\pi} \frac{1}{(c_s(\hat{q}))^3} \equiv \frac{1}{c^2}$$

...mperature

$$\frac{\partial}{\partial T}\left(\frac{1}{V}\sum_{q,s}\right) \frac{\hbar c_s(\hat{q}) q}{e^{\beta \hbar c_s(\hat{q}) q} - 1} = \frac{\partial}{\partial T} \sum_s \int \frac{d\Omega}{4\pi} \int_0^\infty \frac{dx}{2\pi^2} \frac{x^3 \hbar c_s(\hat{q})}{[\beta \hbar c_s(\hat{q})]^4} \frac{1}{e^x - 1}$$

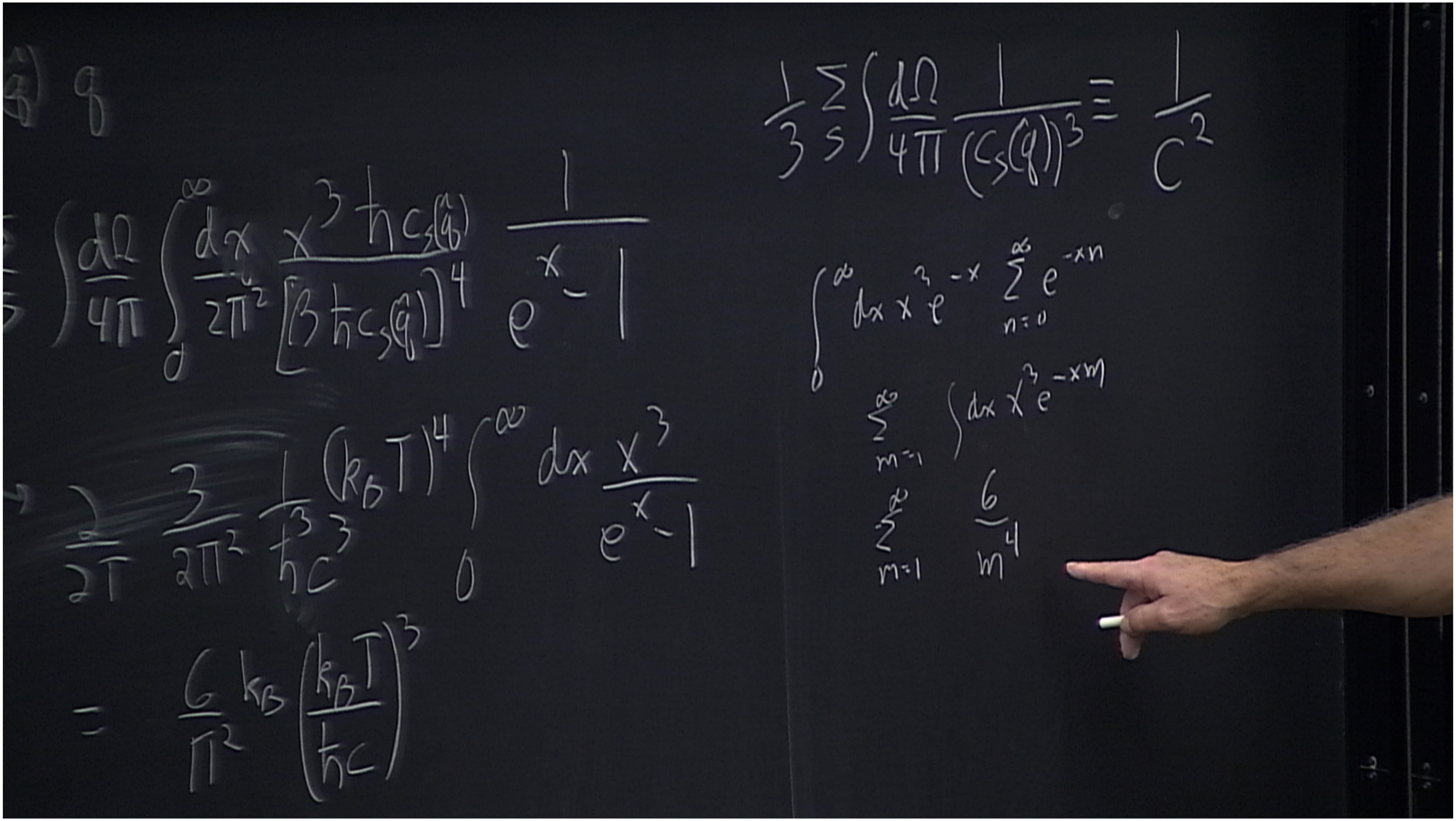
$$\int_0^\infty dx\, x^3 e^{-x} \sum_{n=0}^\infty e^{-xn}$$

$$\sum_{m=1}^\infty \int dx\, x^3 e^{-xm}$$

$$\int \frac{d^3q}{(2\pi)^3} \rightarrow \int_{\text{all angles}} \frac{d\Omega}{4\pi} \int_0^\infty \frac{dq}{2\pi^2} q^2$$

$$\rightarrow \frac{\partial}{\partial T} \frac{3}{2\pi^2} \frac{1}{\hbar^3 c^3} (k_B T)^4 \int_0^\infty dx \frac{x^3}{e^x - 1}$$

$$= \frac{6}{\pi^2} k_B \left(\frac{k_B T}{\hbar c}\right)^3$$



$\frac{1}{3}\sum_s \int \frac{d\Omega}{4\pi} \frac{1}{(c_s(\hat{q}))^3} \equiv \frac{1}{c^2}$
$\int \frac{d\Omega}{4\pi} \int_0^\infty \frac{dx}{2\pi^2} \frac{x^3 \hbar c_s(\hat{q})}{[\beta \hbar c_s(\hat{q})]^4} \frac{1}{e^x - 1}$
$\int_0^\infty dx\, x^3 e^{-x} \sum_{n=0}^\infty e^{-xn}$
$\sum_{m=1}^\infty \int dx\, x^3 e^{-xm}$
$\sum_{m=1}^\infty \frac{6}{m^4}$
$\frac{2}{2T} \frac{3}{2\pi^2} \frac{1}{\hbar^3 c^3} (k_B T)^4 \int_0^\infty dx \frac{x^3}{e^x - 1}$
$= \frac{6}{\pi^2} k_B \left(\frac{k_B T}{\hbar c}\right)^3$

$$\int \frac{d\Omega}{4\pi} \int_0^\infty \frac{dx}{2\pi^2} \frac{x^3\, \hbar c_s(\hat{q})}{[\beta \hbar c_s(\hat{q})]^4} \frac{1}{e^x - 1}$$

$$\frac{\partial}{\partial T} \frac{3}{2\pi^2} \frac{1}{\hbar^3 c^3} (k_B T)^4 \int_0^\infty dx \frac{x^3}{e^x - 1}$$

$$= \frac{6}{\pi^2} k_B \left(\frac{k_B T}{\hbar c}\right)^3 \frac{\pi^4}{15} = \frac{2\pi^2}{5} k_B \left(\frac{k_B T}{\hbar c}\right)^3$$

$$\frac{1}{3} \sum_s \int \frac{d\Omega}{4\pi} \frac{1}{(c_s(\hat{q}))^3} \equiv \frac{1}{c^2}$$

$$\int_0^\infty dx\, x^3 e^{-x} \sum_{n=0}^\infty e^{-xn}$$

$$\sum_{m=1}^\infty \int dx\, x^3 e^{-xm}$$

$$\sum_{m=1}^\infty \frac{6}{m^4} = \frac{\pi^4}{15}$$

Einstein (1907) assume $\omega_s(q) = \omega_E$

" there are 'p' such modes

Einstein (1907)   assume $\omega_s(q) = \omega_E$

" there are 'p' such modes

$$\frac{1}{V}\sum_{qs} 1 = p\frac{N}{V} = pn$$

$$c_V = pn\,\hbar\omega_E\,(-)\,1\,\frac{-\frac{\hbar\omega_E}{(k_B T)^2}\cdot k_B\, e^{\hbar\omega_E/k_BT}}{\left(e^{\hbar\omega_E/k_BT}-1\right)^2} = pn\,\hbar \ldots$$

assume $\omega_s(q) = \omega_E$

" there are 'p' such modes

$$\frac{1}{V}\sum_{qs} 1 = p\frac{N}{V} = pn$$

$$c_V = pn\,\hbar\omega_E(-)\frac{1}{\left(e^{\hbar\omega_E/k_BT}-1\right)^2}\cdot\frac{-\hbar\omega_E\cdot k_B}{(k_BT)^2}\,e^{\hbar\omega_E/k_BT} = pn\left(\frac{\hbar\omega_E}{k_BT}\right)^2\frac{e^{\hbar\omega_E/k_BT}}{\left(e^{\hbar\omega_E/k_BT}-1\right)^2}$$

sume $\omega_s(q) = \omega_E$

" there are 'p' such modes

$$\frac{1}{V}\sum_{qs} 1 = p\frac{N}{V} = pn$$

$$pn\,\hbar\omega_E \frac{(-)\,1}{\left(e^{\hbar\omega_E/k_BT}-1\right)^2}\,\frac{-\hbar\omega_E\cdot k_B}{(k_BT)^2}\, e^{\hbar\omega_E/k_BT} = pn\left(\frac{\hbar\omega_E}{k_BT}\right)^2\frac{e^{\hbar\omega_E/k_BT}}{\left(e^{\hbar\omega_E/k_BT}-1\right)^2} \sim \frac{1}{T^2}e^{-\frac{\hbar\omega_E}{k_BT}}$$

Debye (1912): $\omega_s(\vec{q}) = cq$ for 3 acoustic modes, c is independent of s.

for $q < q_D$

$-\frac{\hbar\omega_E}{k_B T}$

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for $q < q_D$

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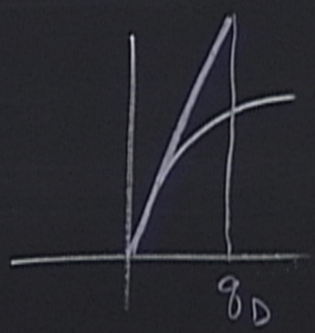
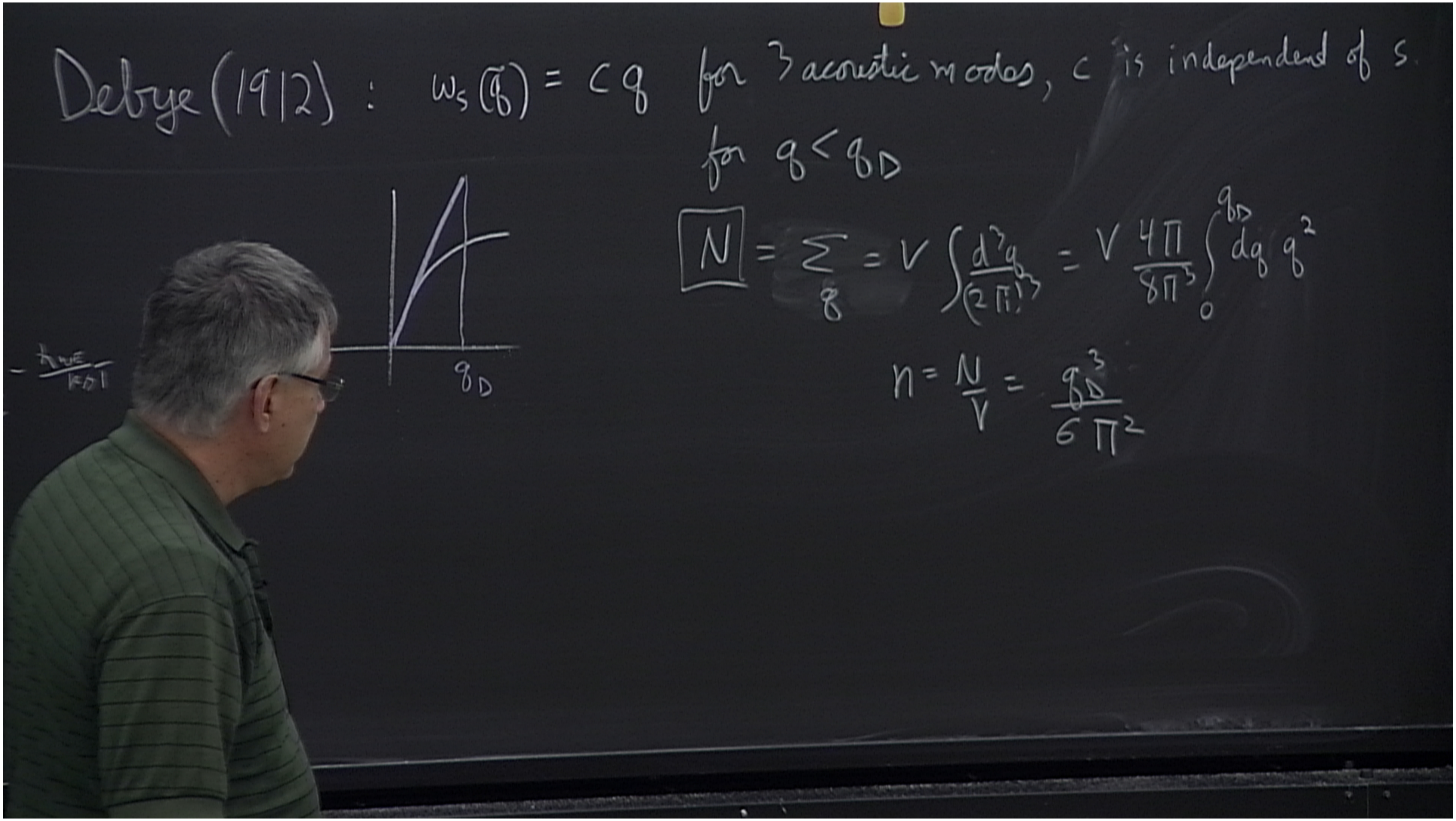
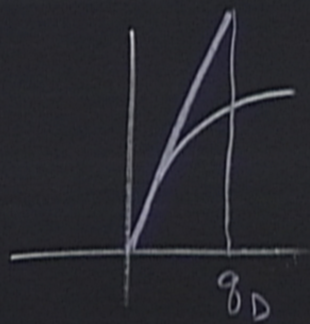



Debye (1912) : ωs(q) = cq for 3 acoustic modes, c is independent of s.
for q < qD
N = Σq = V ∫ d³q/(2π)³ = V 4π/8π³ ∫0^qD dq q²
n = N/V = qD³/6π²
qD

Debye (1912): $\omega_s(\vec{q}) = cq$ for 3 acoustic modes, c is independent of s.

for $q < q_D$

$-\frac{\hbar\omega_E}{k_B T}$



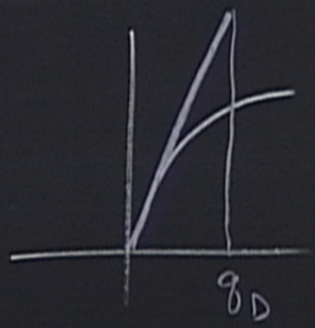
$$\boxed{N} = \sum_{q} = V\int \frac{d^3q}{(2\pi)^3} = V\frac{4\pi}{8\pi^3}\int_0^{q_D} dq\, q^2$$

$$n = \frac{N}{V} = \frac{q_D^3}{6\pi^2} \Rightarrow q_D = (6\pi^2 n)^{\frac{1}{3}}$$

Debye (1912) : $\omega_s(\vec{q}) = cq$ for 3 acoustic modes, c is independent of s.

for $q < q_D$

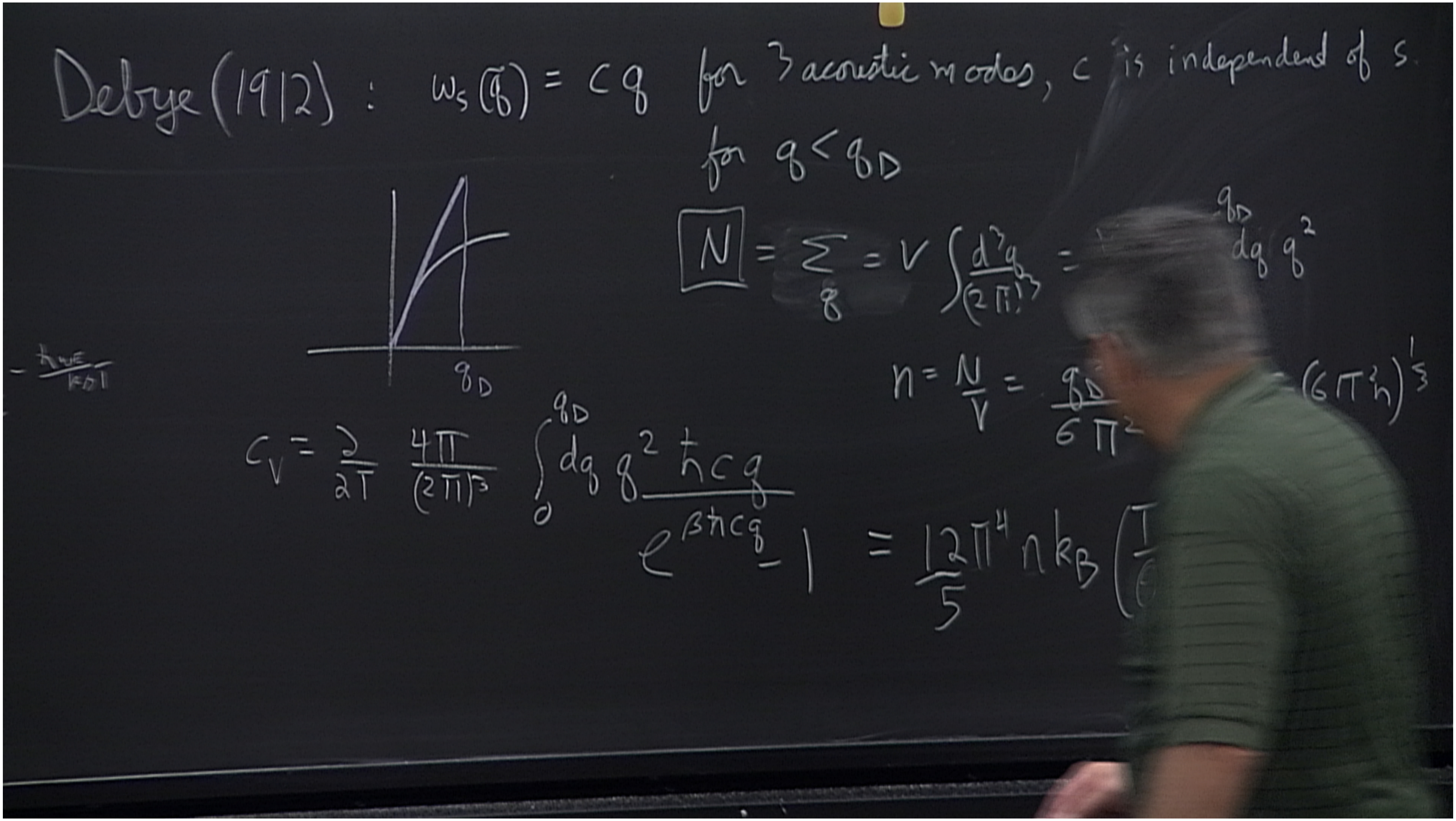
$-\frac{\hbar\omega_E}{k_B T}$



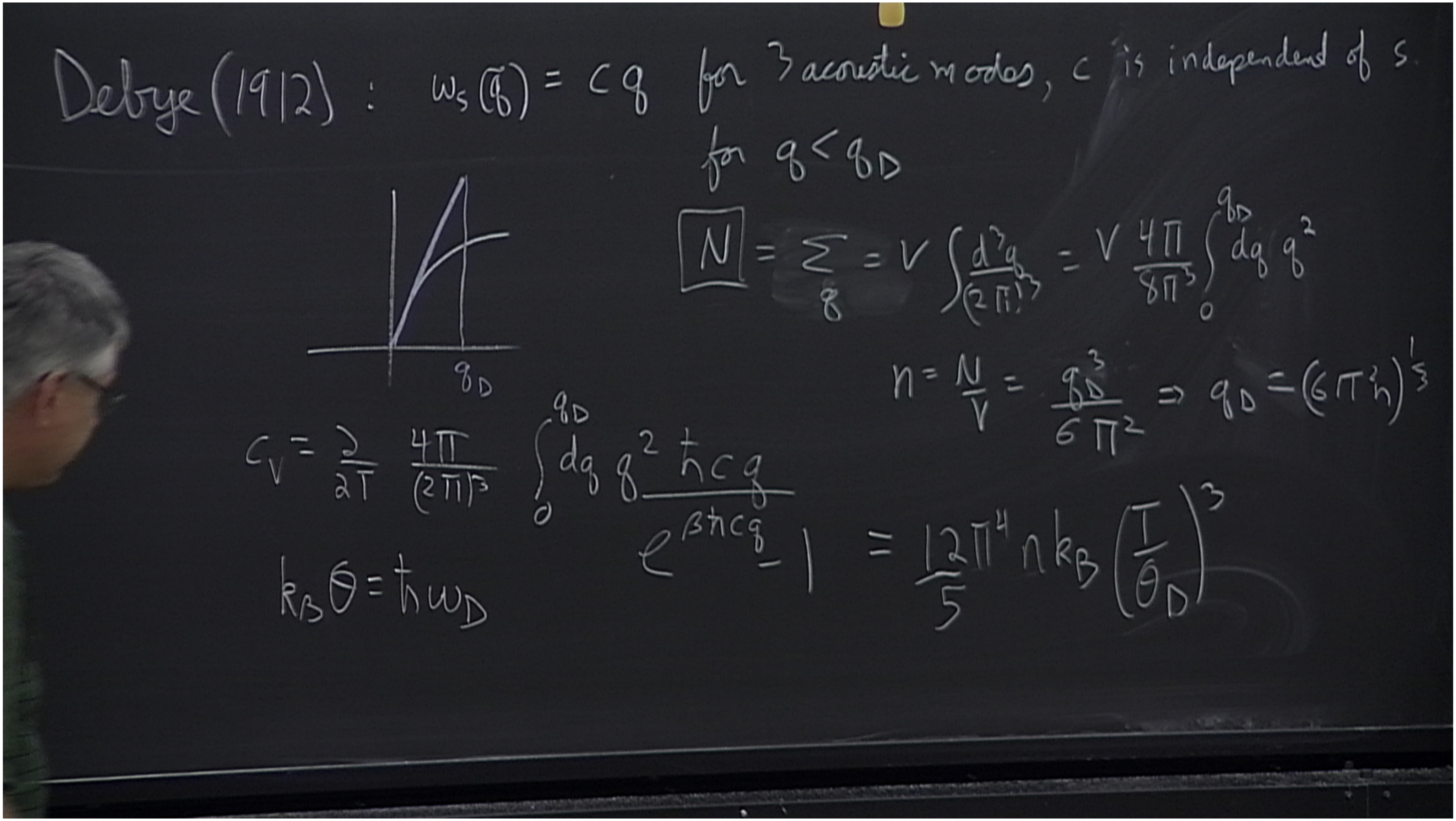
$$\boxed{N} = \sum_{q} = V\int\frac{d^3q}{(2\pi)^3} = V\,\frac{4\pi}{8\pi^3}\int_0^{q_D} dq\, q^2$$

$$n = \frac{N}{V} = \frac{q_D^3}{6\pi^2} \Rightarrow q_D = (6\pi^2 n)^{\frac{1}{3}}$$

$$C_V = \frac{\partial}{\partial T}\,\frac{4\pi}{(2\pi)^3}\int_0^{q_D} dq\, q^2\,\frac{\hbar c q}{e^{\beta\hbar c q} - 1}$$

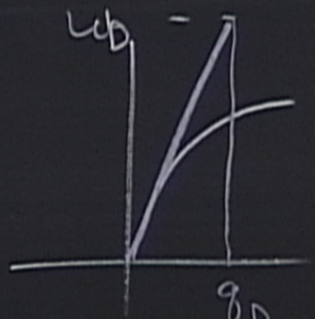


Debye (1912) : $\omega_s(\vec{q}) = cq$ for 3 acoustic modes, c is independent of s.
for $q < q_D$
$\boxed{N} = \sum_q = V \int \frac{d^3q}{(2\pi)^3} =$
$dq\, q^2$
q_D
$n = \frac{N}{V} = \frac{q_D}{6\pi^2}$
$(6\pi^2 n)^{\frac{1}{3}}$
$c_V = \frac{\partial}{\partial T} \frac{4\pi}{(2\pi)^3} \int_0^{q_D} dq\, q^2 \frac{\hbar c q}{e^{\beta \hbar c q} - 1} = \frac{12\pi^4}{5} n k_B \Big($


Debye (1912) : $\omega_s(\vec{q}) = cq$ for 3 acoustic modes, c is independent of s.
for $q < q_D$
q_D
$\boxed{N} = \sum_q = V\int \frac{d^3q}{(2\pi)^3} = V\frac{4\pi}{8\pi^3}\int_0^{q_D} dq\, q^2$
$n = \frac{N}{V} = \frac{q_D^3}{6\pi^2} \Rightarrow q_D = (6\pi^2 n)^{\frac{1}{3}}$
$c_V = \frac{\partial}{\partial T}\frac{4\pi}{(2\pi)^3}\int_0^{q_D} dq\, q^2 \frac{\hbar c q}{e^{\beta\hbar c q}-1} = \frac{12}{5}\pi^4 n k_B \left(\frac{T}{\Theta_D}\right)^3$
$k_B\Theta = \hbar\omega_D$

Debye (1912) : $\omega_s(\vec{q}) = cq$ for 3 acoustic modes, c is independent of s.

for $q < q_D$



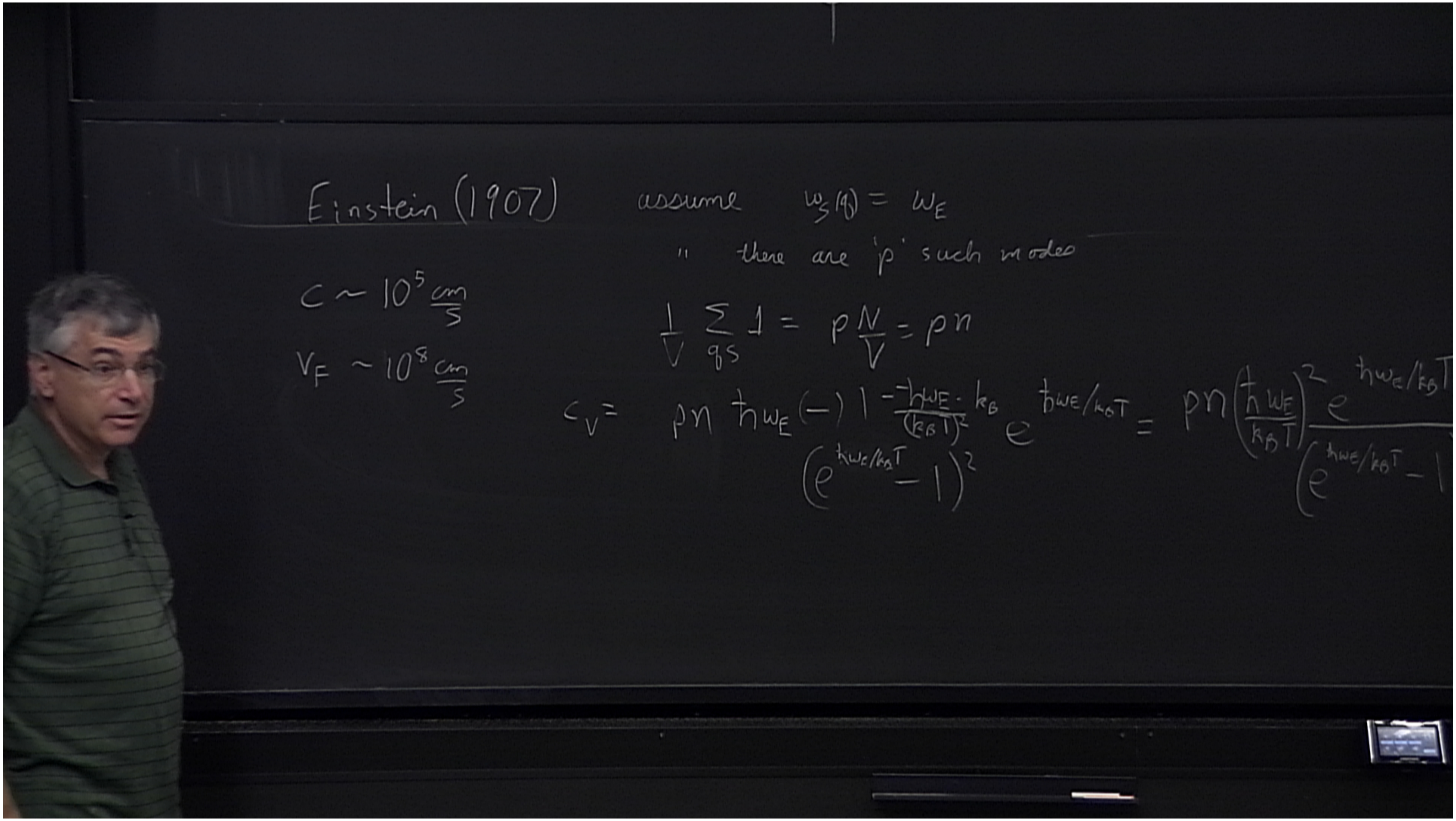
$-\frac{\hbar\omega_E}{k_B T}$

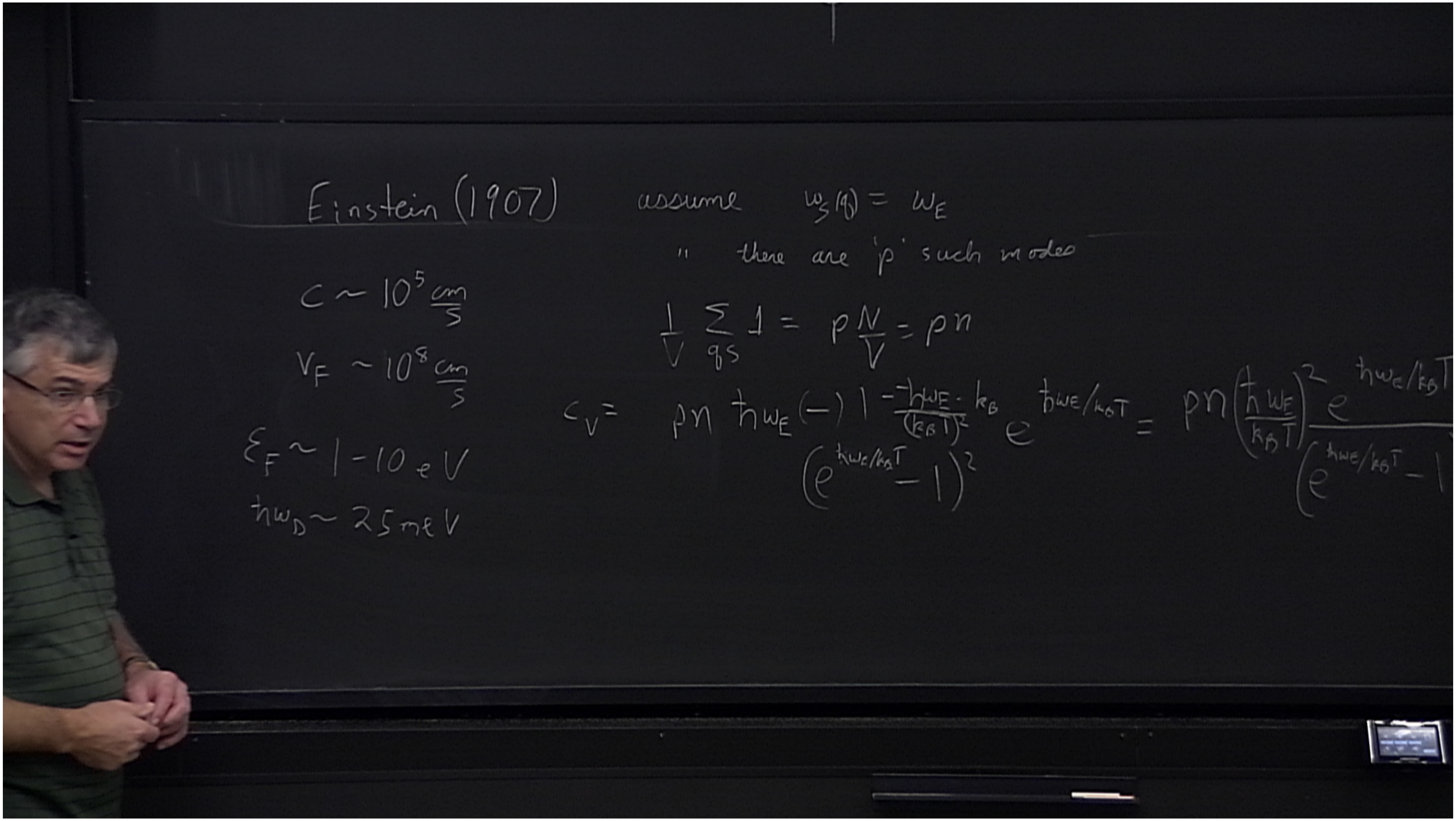
$$\boxed{N} = \sum_{q} = V\int\frac{d^3q}{(2\pi)^3} = V\frac{4\pi}{8\pi^3}\int_0^{q_D} dq\, q^2$$

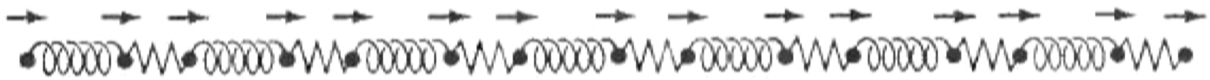
$$n = \frac{N}{V} = \frac{q_D^3}{6\pi^2} \Rightarrow q_D = (6\pi^2 n)^{\frac{1}{3}}$$

$$c_V = \frac{\partial}{\partial T}\frac{4\pi}{(2\pi)^3}\int_0^{q_D} dq\, q^2\frac{\hbar c q}{e^{\beta\hbar c q}-1} = \frac{12\pi^4}{5} n k_B\left(\frac{T}{\Theta_D}\right)^3$$

$$k_B\Theta_D = \hbar\omega_D \equiv \hbar c q_D$$


Einstein (1907)
assume $\omega_s(q) = \omega_E$
" there are 'p' such modes
$c \sim 10^5 \frac{cm}{s}$
$v_F \sim 10^8 \frac{cm}{s}$
$\frac{1}{V}\sum_{qs} 1 = p\frac{N}{V} = pn$
$c_V = pn\,\hbar\omega_E \frac{(-)\,1}{\left(e^{\hbar\omega_E/k_BT}-1\right)^2} \frac{-\hbar\omega_E}{(k_BT)^2}\cdot k_B\, e^{\hbar\omega_E/k_BT} = pn\left(\frac{\hbar\omega_E}{k_BT}\right)^2 \frac{e^{\hbar\omega_E/k_BT}}{\left(e^{\hbar\omega_E/k_BT}-1\right.}$


Einstein (1907)
$c \sim 10^5 \frac{cm}{s}$
$v_F \sim 10^8 \frac{cm}{s}$
$\varepsilon_F \sim 1-10\ eV$
$\hbar\omega_D \sim 25\ meV$
assume $\omega_s(q) = \omega_E$
" there are 'p' such modes
$\frac{1}{V}\sum_{qs} 1 = p\frac{N}{V} = pn$
$c_V = pn\,\hbar\omega_E \frac{(-)\,1 \cdot -\frac{\hbar\omega_E}{(k_B T)^2} \cdot k_B\, e^{\hbar\omega_E/k_BT}}{(e^{\hbar\omega_E/k_BT}-1)^2} = pn\left(\frac{\hbar\omega_E}{k_BT}\right)^2 \frac{e^{\hbar\omega_E/k_BT}}{(e^{\hbar\omega_E/k_BT}-1)}$



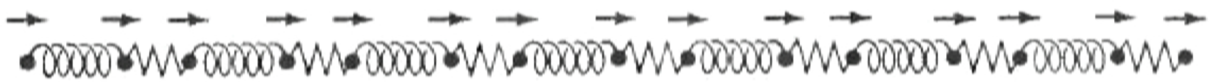
(a)

(b)

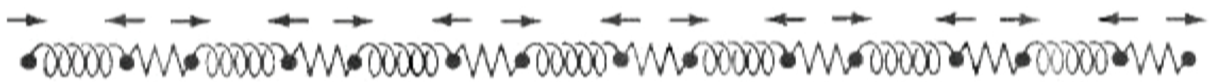
Figure 22.11

The long wavelength acoustic (a) and optical (b) modes in the diatomic linear chain. The primitive cell contains the two ions joined by the K-spring, represented by a jagged line. In both cases the motion of every primitive cell is identical, but in the acoustic mode the ions within a cell move together, while they move 180° out of phase in the optical mode.

Ashcroft and Mermin Fig. 22.11



(a)



(b)

Figure 22.11
The long wavelength acoustic (a) and optical (b) modes in the diatomic linear chain. The primitive cell contains the two ions joined by the K-spring, represented by a jagged line. In both cases the motion of every primitive cell is identical, but in the acoustic mode the ions within a cell move together, while they move 180° out of phase in the optical mode.

Ashcroft and Mermin Fig. 22.11

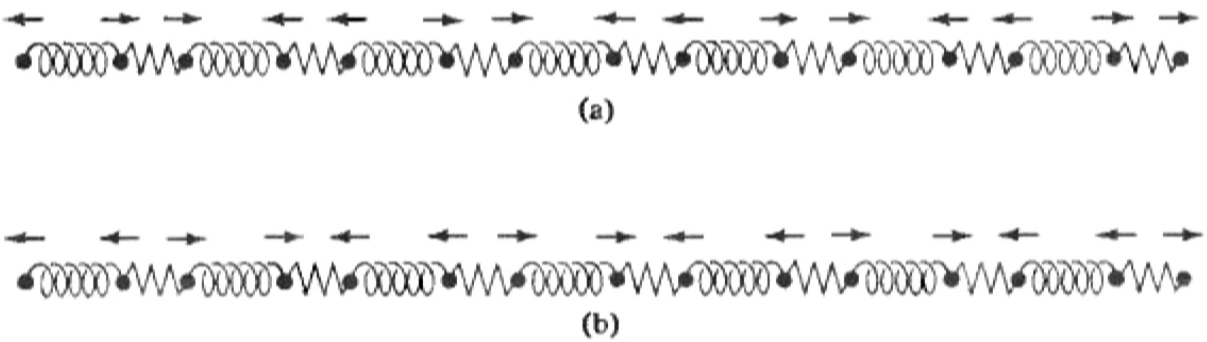
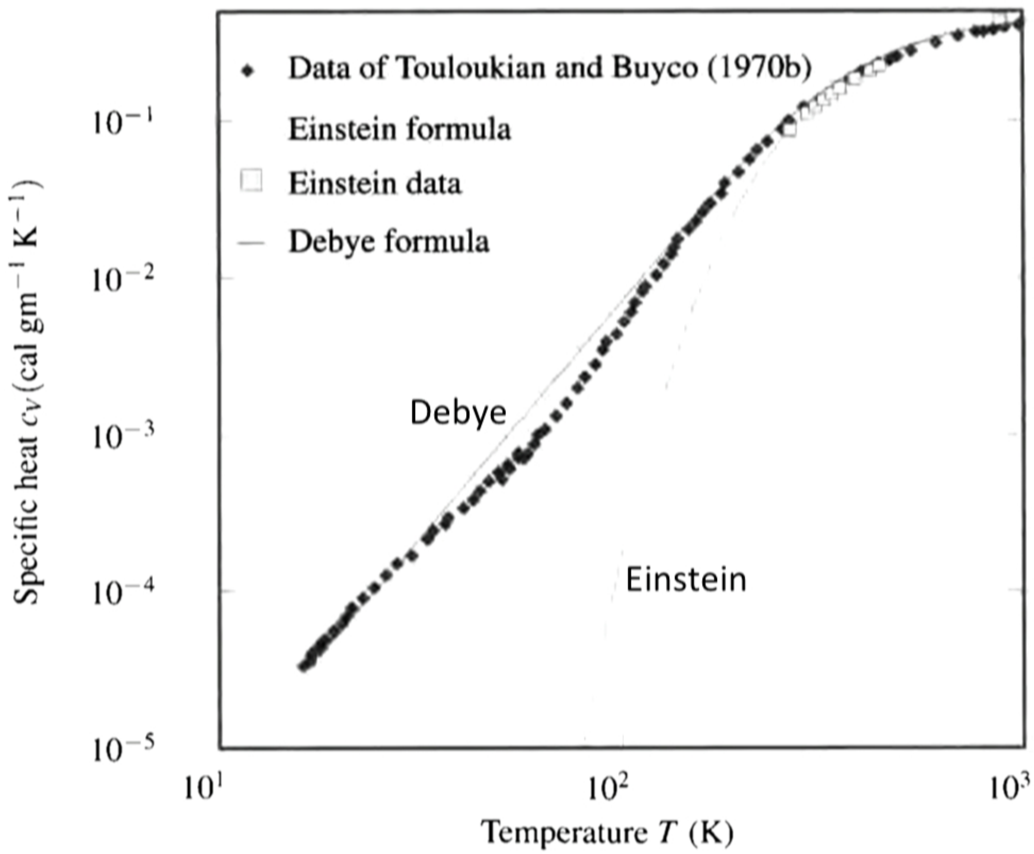


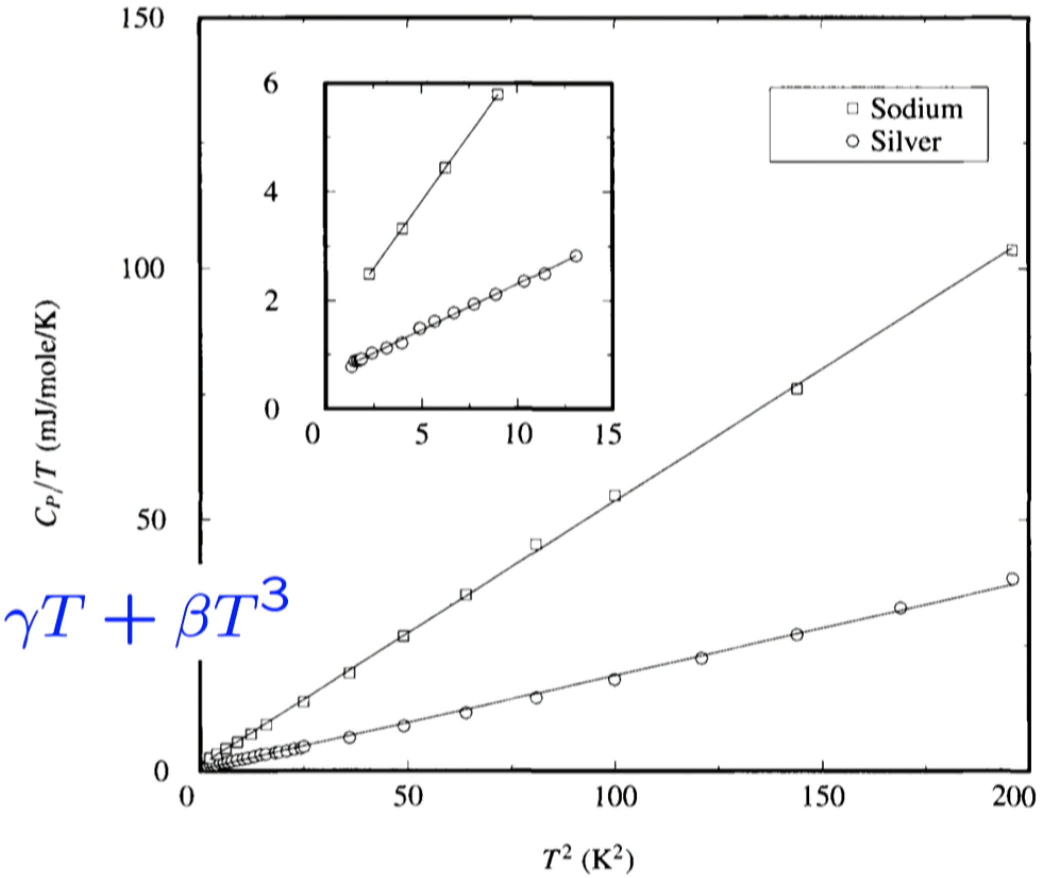
Figure 22.12
The acoustic (a) and optical (b) modes of the diatomic linear chain, when $k = \pm\pi/a$, at the edges of the Brillouin zone. Now the motion changes by 180° from cell to cell. However, as in Figure 22.11, the ions within each cell move in phase in the acoustic mode, and 180° out of phase in the optical mode. Note that if the K- and G-springs were identical the motion would be the same in both cases. This is why the two branches become degenerate at the edges of the zone when $K = G$.

Ashcroft and Mermin Fig. 22.12

Quantum Lattice Vibrations: phonons

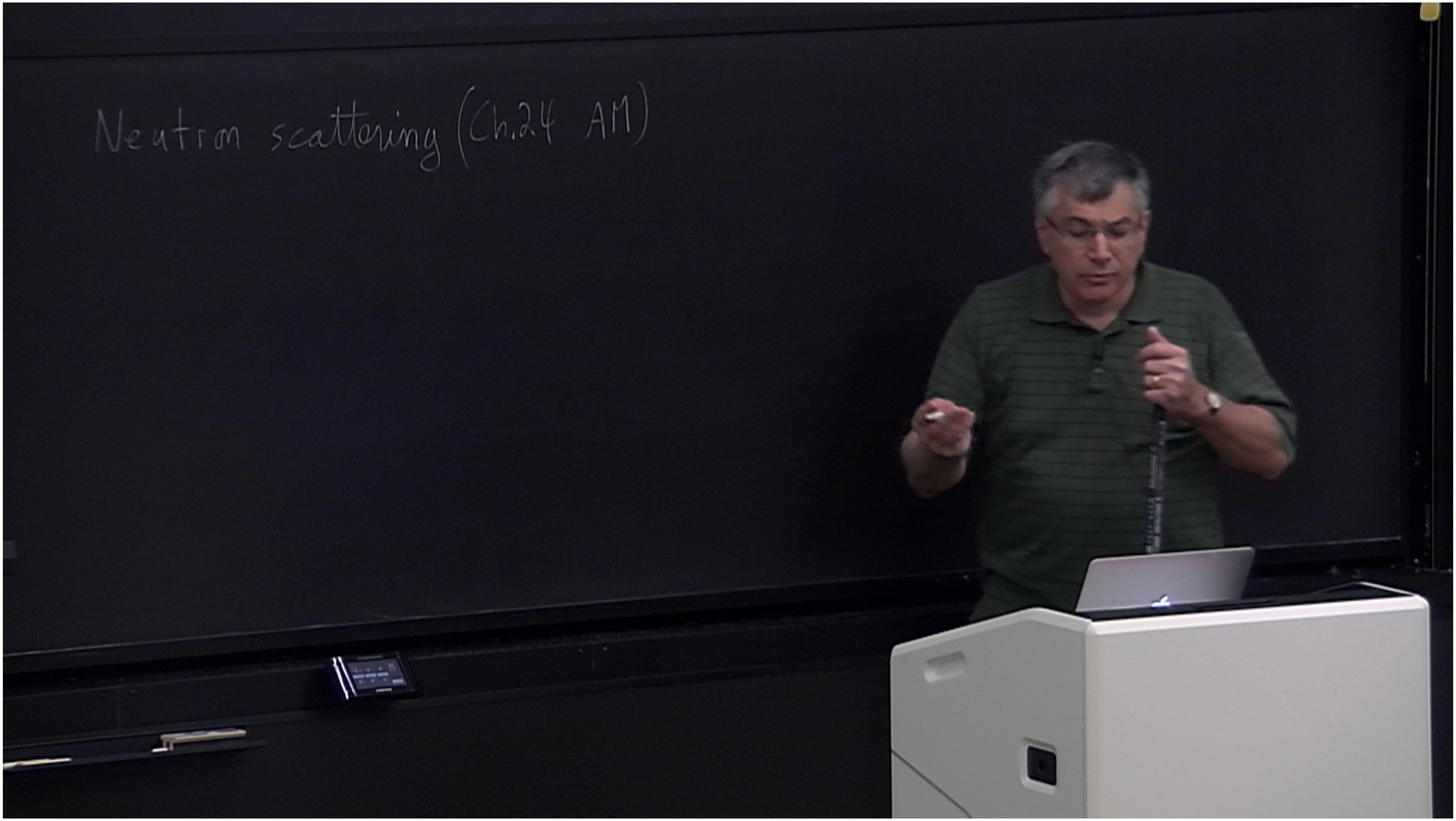


M. Marder, Condensed Matter Physics (2nd ed. 2010) Fig. 13.8



$$C_V = \gamma T + \beta T^3$$

M. Marder, Condensed Matter Physics (2nd ed. 2010) Fig. 13.11


Neutron scattering (Ch.24 AM)

Neutron vs photon dispersion curves

Figure 24.1
Neutron (n) and photon (γ) energy-momentum relations. When $k = 10^n$ cm^{-1}, $E_n = 2.07 \times 10^{2n-19}$ eV and $E_\gamma = 1.97 \times 10^{n-5}$ eV. Typical thermal energies lie in or near the white band.

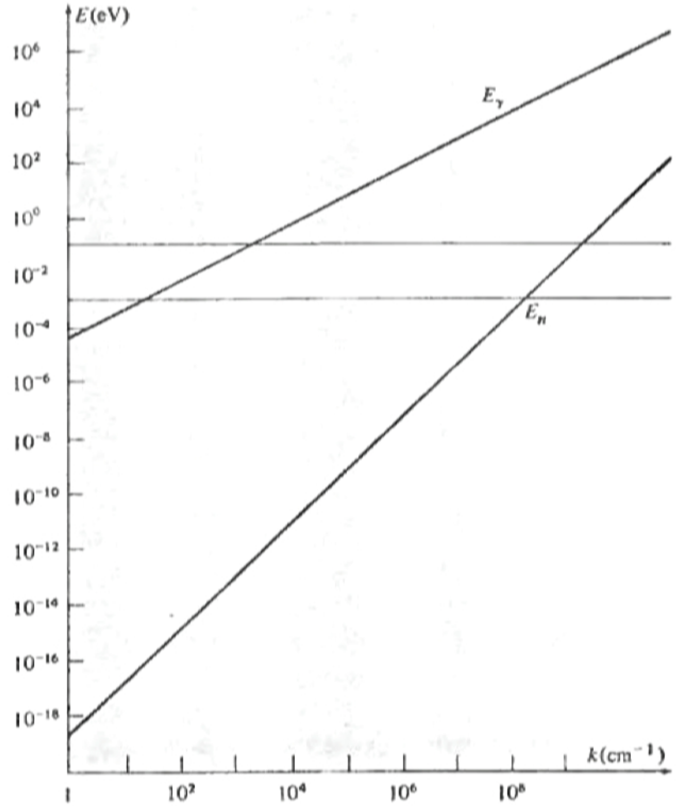
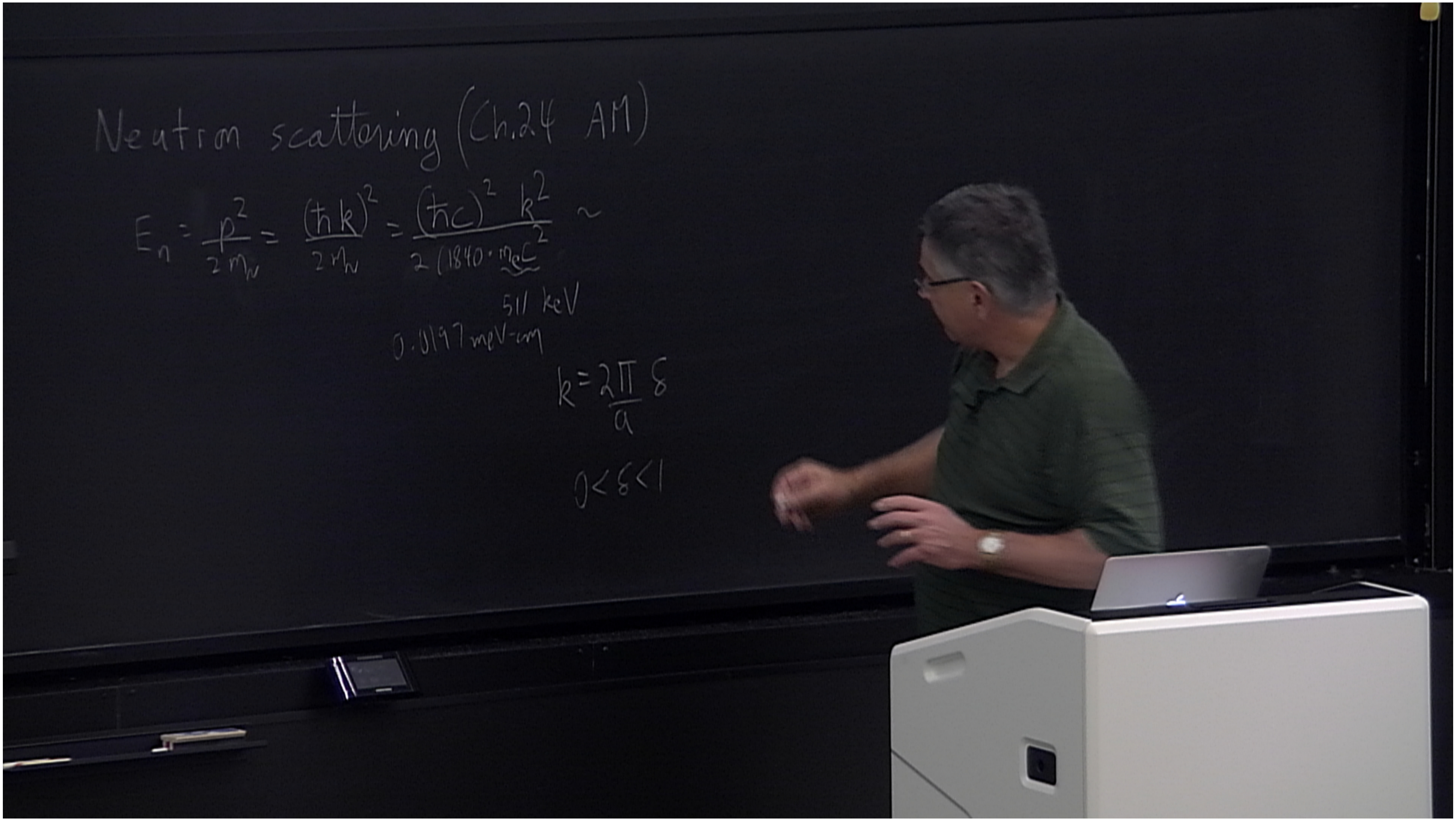
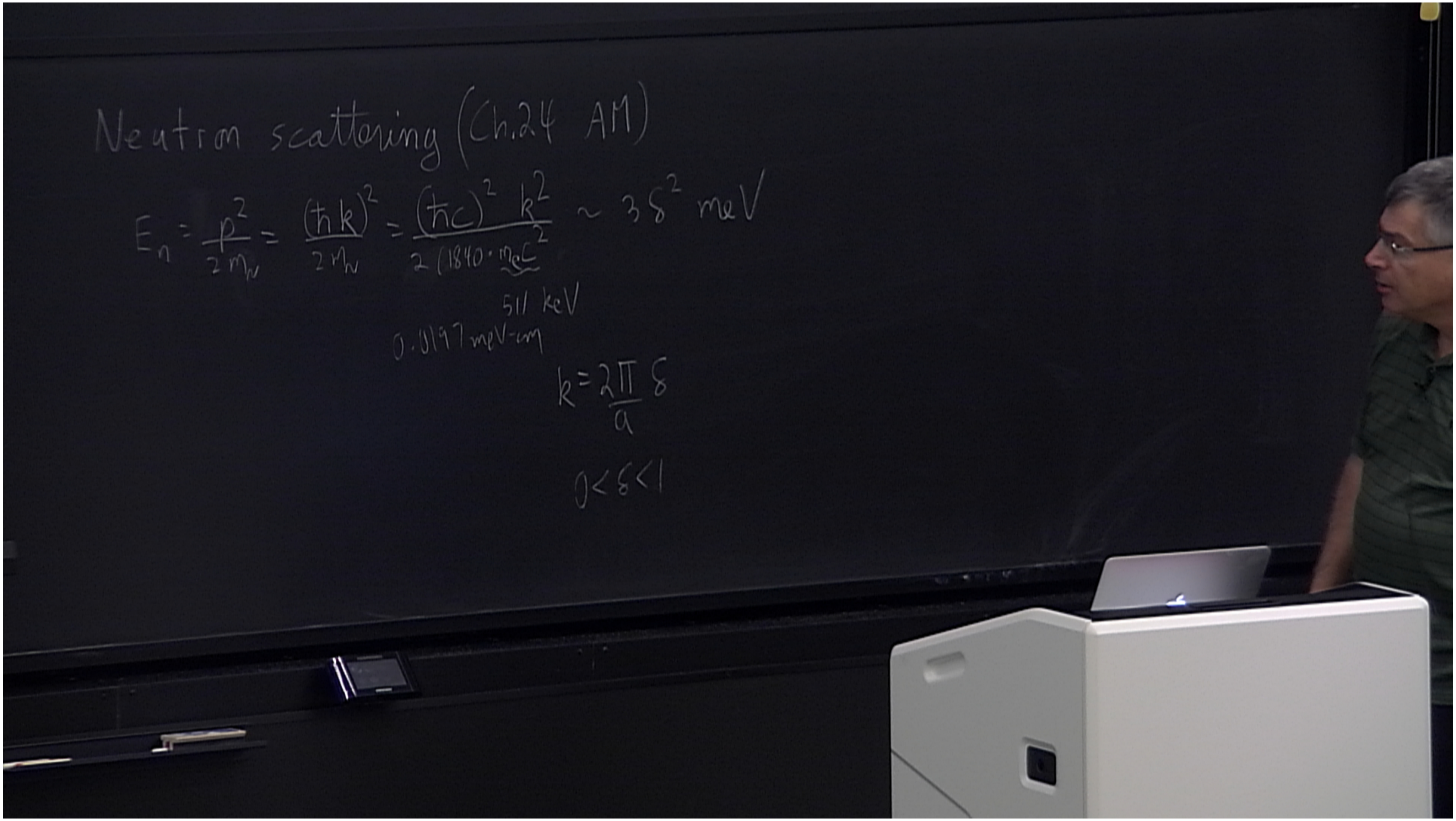
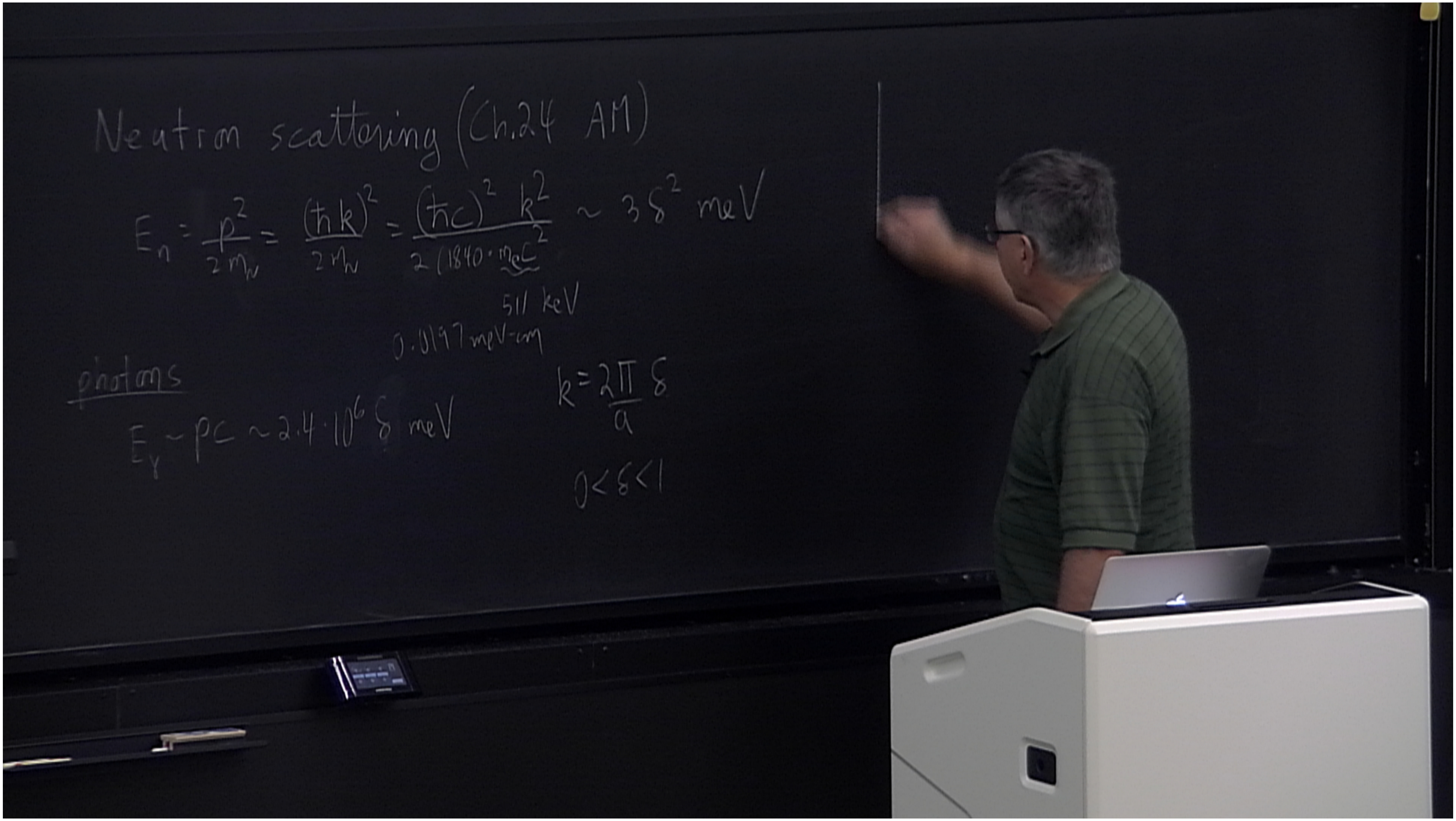


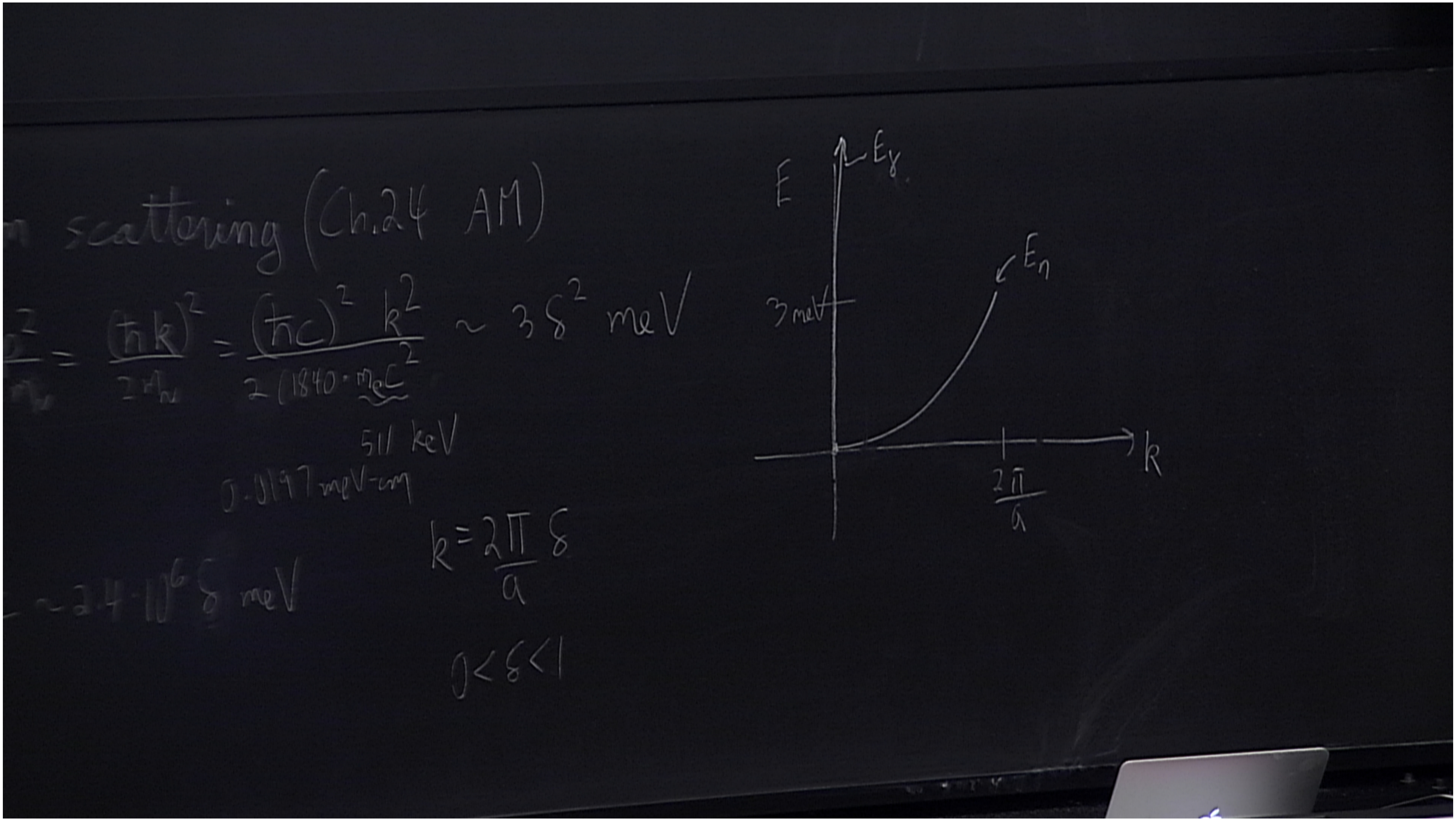
Fig. 24.1 from Ashcroft and Mermin


Neutron scattering (Ch.24 AM)
En = p^2/2mN = (ħk)^2/2mN = (ħc)^2 k^2 / 2(1840·mec^2) ~
511 keV
0.0197 meV-cm
k = 2π/a δ
0 < δ < 1


Neutron scattering (Ch.24 AM)
E_n = p^2/2m_N = (ħk)^2/2m_N = (ħc)^2 k^2 / 2(1840 · m_e c^2) ~ 3δ^2 meV
511 keV
0.0197 meV-cm
k = 2π/a δ
0 < δ < 1


Neutron scattering (Ch.24 AM)
$E_n = \frac{p^2}{2m_N} = \frac{(\hbar k)^2}{2m_N} = \frac{(\hbar c)^2 k^2}{2(1840 \cdot m_e c^2)} \sim 3\delta^2$ meV
511 keV
0.0197 meV-cm
photons
$E_\gamma \sim pc \sim 2.4 \cdot 10^6 \delta$ meV
$k = \frac{2\pi}{a} \delta$
$0 < \delta < 1$

E
E_γ
E_n
3 meV
meV
k
$\frac{2\pi}{a}$


scattering (Ch.24 AM)
(ħk)^2 / 2M_n = (ħc)^2 k^2 / 2(1840 · m_e c^2) ~ 3 δ^2 meV
511 keV
0.1197 meV-cm
~ 2.4 · 10^6 δ meV
k = 2π/a δ
0 < δ < 1
E
E_γ
E_n
3 meV
k
2π/a

R.M. White, Quantum Theory of Magnetism

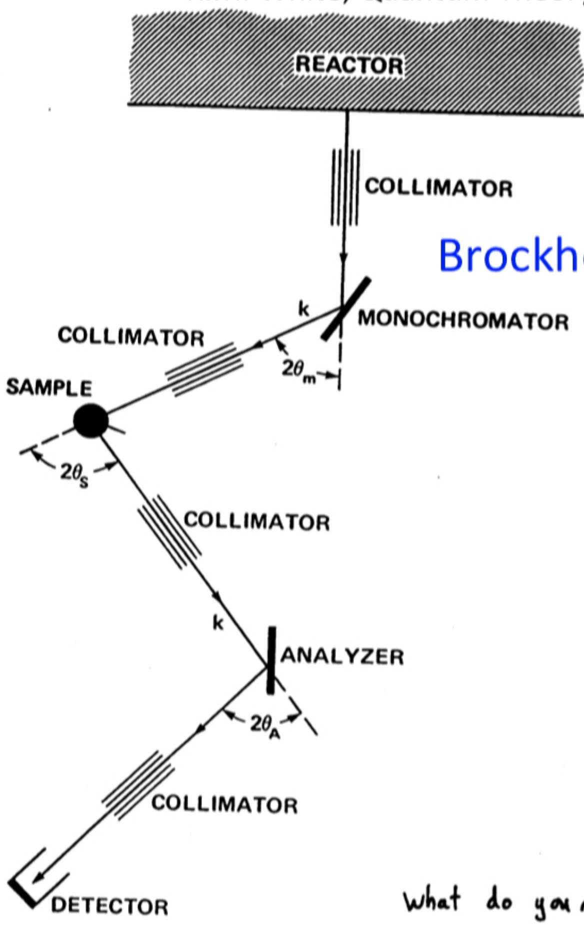


Fig. 8.2. Schematic diagram of a triple-axis spectrometer

Brockhouse

Brockhouse Triple Axis Spectrometer

nuclear scattering

magnetic "

Bragg:

$$\boxed{n\lambda = 2d\sin\theta}$$

What do you measure?

Ans: $S(Q,\omega)$

energy transfer

momentum transfer


Hudson Bay
Baie d'Hudson
James Bay
Baie James
CANADA
ONTARIO
MANITOBA
QUEBEC / QUÉBEC
USA / É-U d'A
UNITED STATES OF AMERICA
ÉTATS-UNIS D'AMÉRIQUE
L Superior
L Supérieur
L Michigan
L Huron
L Ontario
L Erie
L Érié
Ottawa R / R des Outaouais
LEGEND / LEGENDE
National capital / Capitale nationale
Provincial capital / Capitale provinciale
Other populated places / Autres lieux habités
Trans-Canada Highway / La Transcanadienne
Major road / Route principale
International boundary / Frontière internationale
Provincial boundary / Limite provinciale
Scale / Échelle
Ottawa
Toronto
Thunder Bay
Sault Ste Marie
Greater Grand Sudbury
Kingston
Windsor
London
Hamilton


Hudson Bay
Baie d'Hudson
Fort Severn
Peawanuck
MANITOBA
James Bay
Baie James
Big Trout Lake
Attawapiskat
Sandy Lake
Lansdowne House
Moosonee
Pikangikum
ONTARIO
QUEBEC / QUÉBEC
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Red Lake
Sioux Lookout
Armstrong
Kapuskasing
Cochrane
Kenora
Dryden
L Nipigon
Geraldton
Iroquois Falls
Timmins
Marathon
Kirkland Lake
Fort Frances
Thunder Bay
New Liskeard
Wawa
Chapleau
L Superior
L Supérieur
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Hawkesbury
Sault Ste Marie
Elliot Lake
Espanola
Pembroke
Ottawa
Cornwall
Little Current
Huntsville
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Parry Sound
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Kitchener
St Catharines
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Welland
London
Sarnia
St Thomas
Chatham-Kent
Windsor
L Erie
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L Michigan
L Huron
UNITED STATES OF AMERICA
ÉTATS-UNIS D'AMÉRIQUE
CANADA
LEGEND / LEGENDE
National capital / Capitale nationale
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Trans-Canada Highway / La Transcanadienne
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International boundary / Frontière internationale
Provincial boundary / Limite provinciale
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100 0 100 200 300
km
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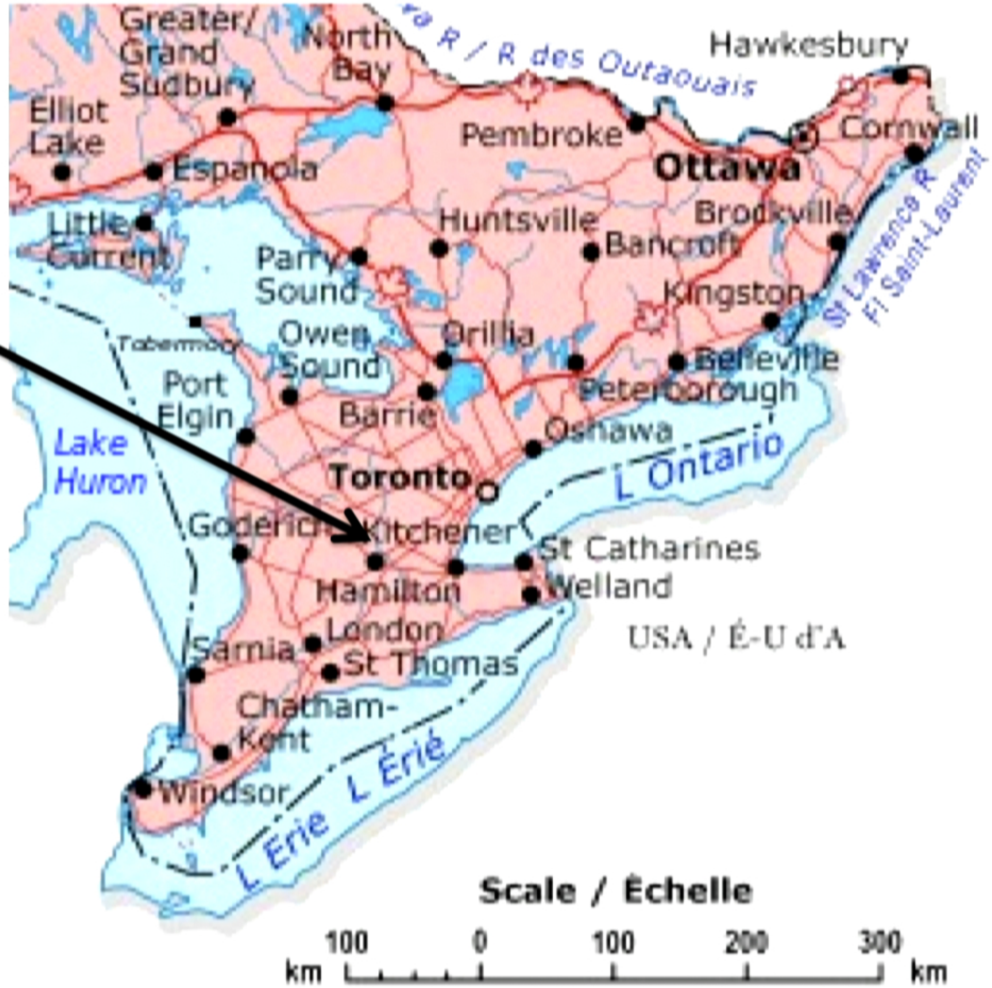
Sa Majesté la Reine du chef du Canada, Ressources naturelles Canada.

We are here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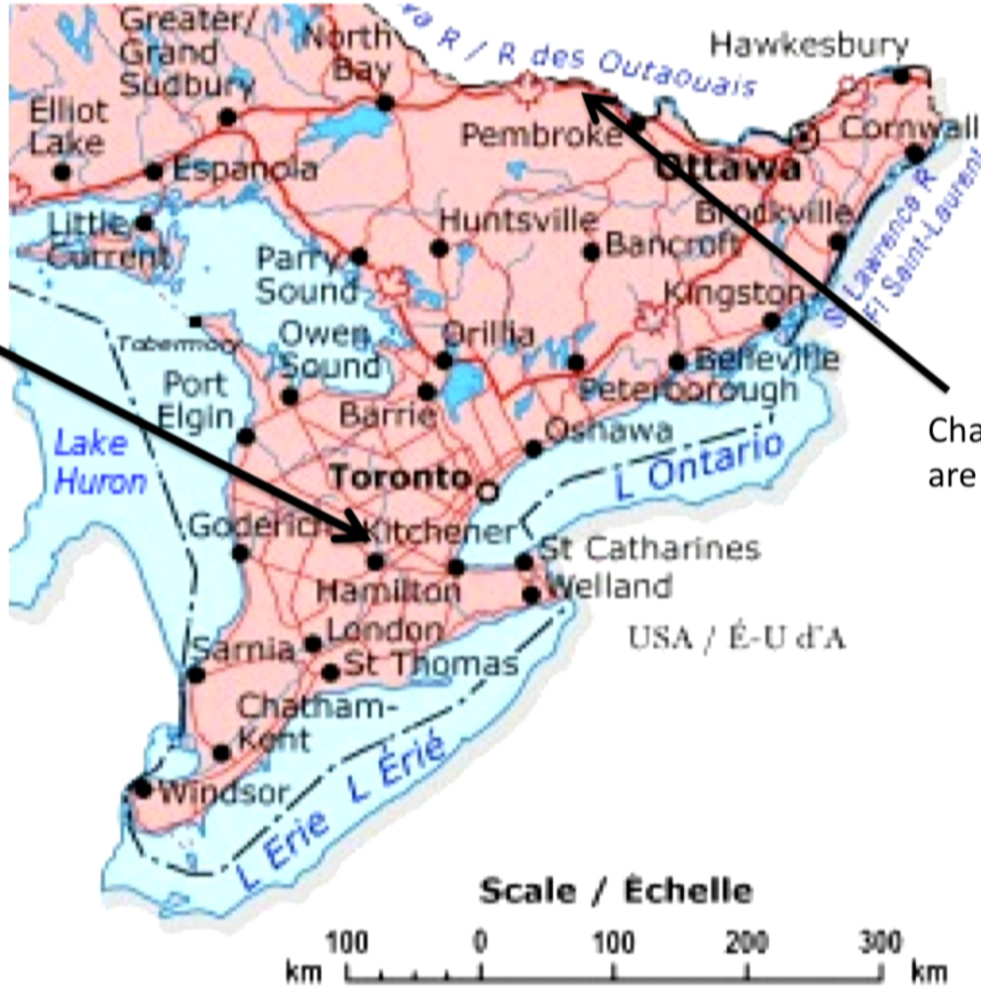
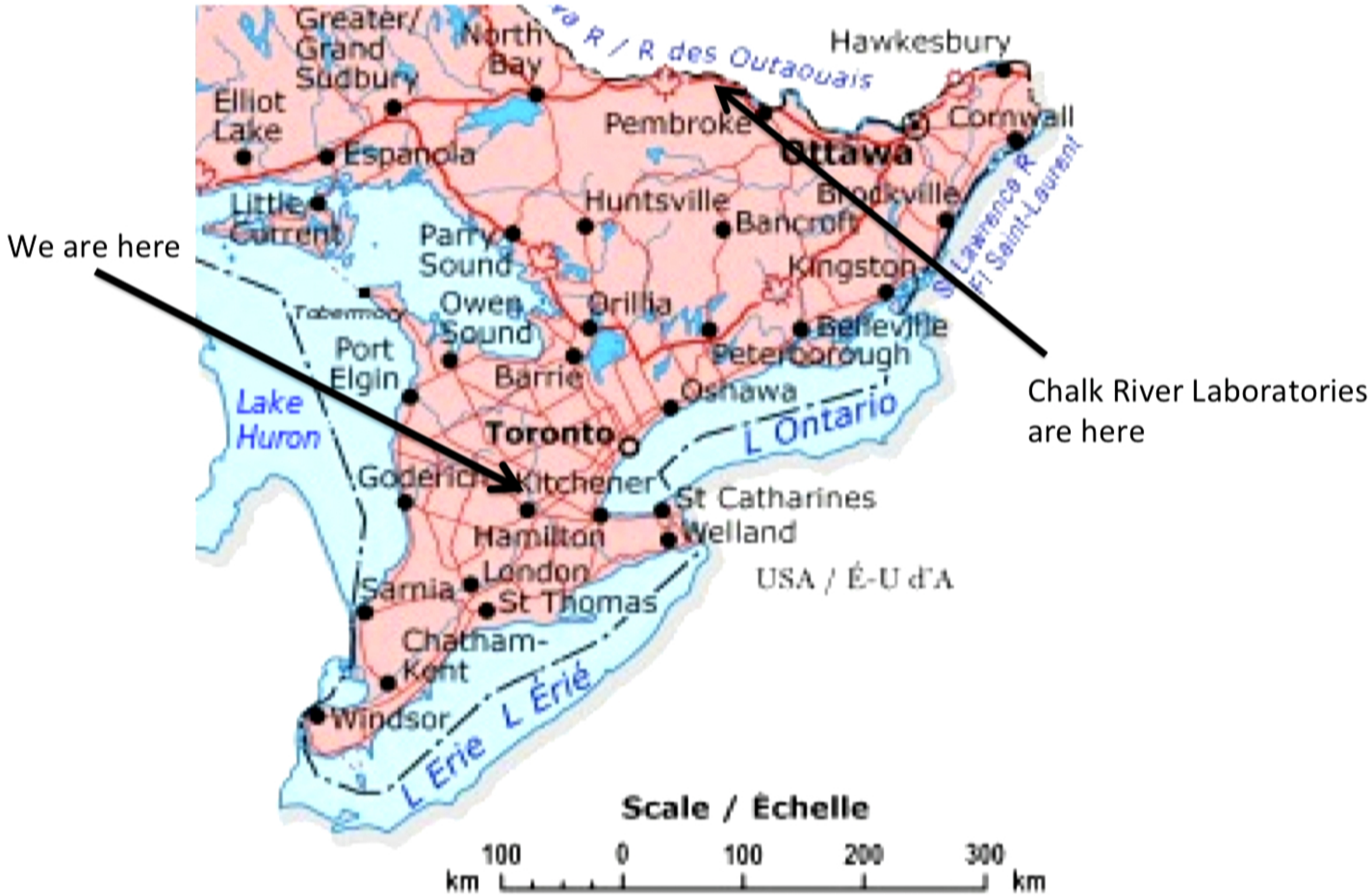


Chalk River Laboratories are here


We are here
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Kent
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Scale / Échelle
100 km 0 100 200 300 km

R.M. White, Quantum Theory of Magnetism

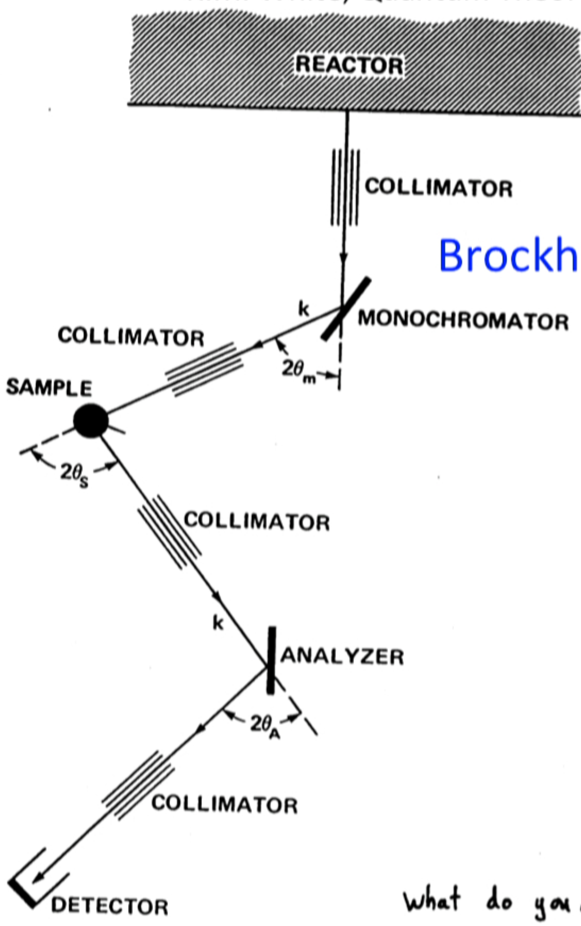

Fig. 8.2. Schematic diagram of a triple-axis spectrometer

Brockhouse

Brockhouse Triple Axis Spectrometer

nuclear scattering

magnetic "

Bragg:

$$\boxed{n\lambda = 2d\sin\theta}$$

What do you measure?

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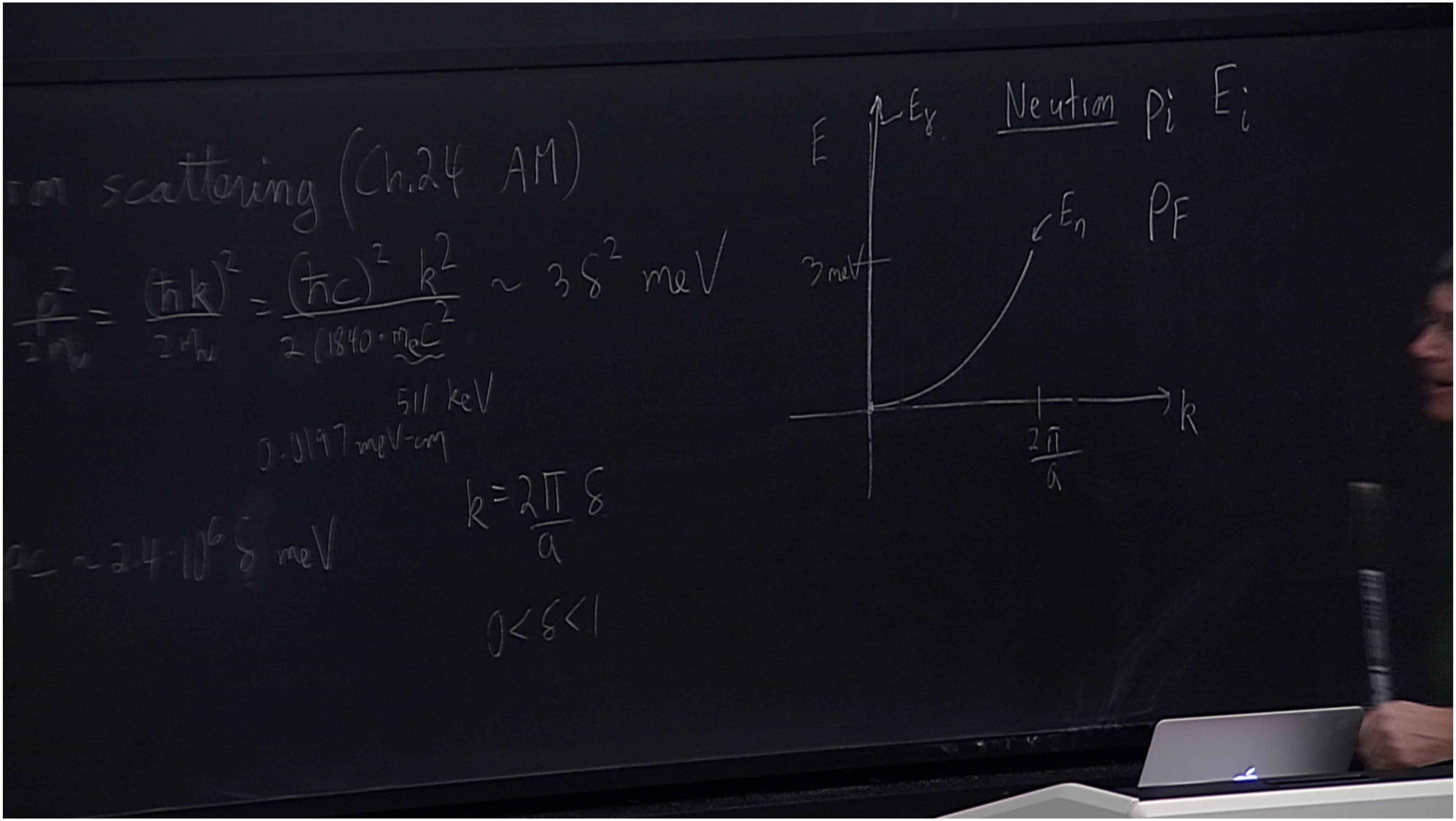
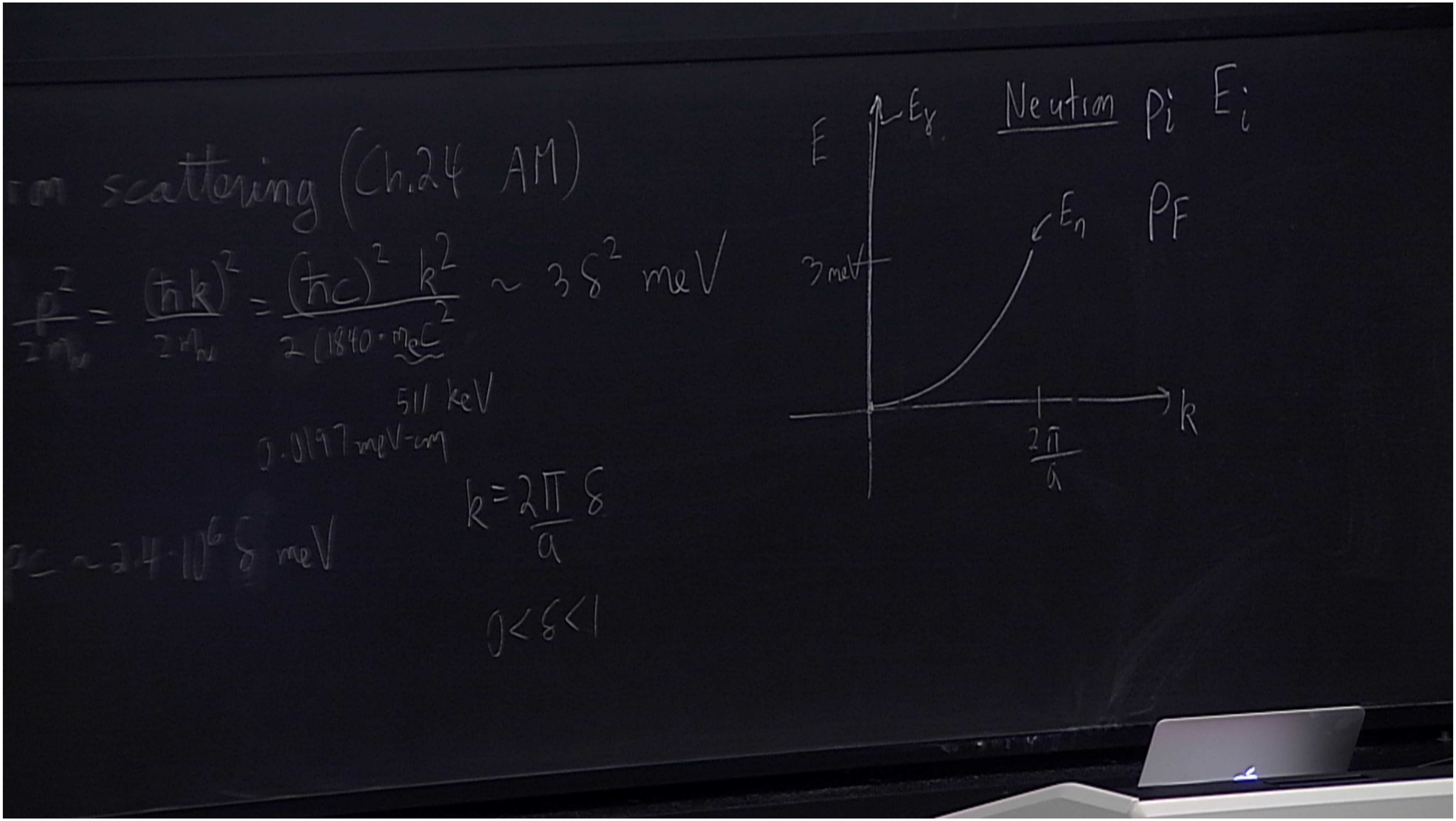
momentum transfer


scattering (Ch.24 AM)
Neutron pi Ei
E
Eγ
En
pF
3 meV
k
2π/a
511 keV
0.0197 meV-cm
k = 2π/a δ
0<δ<1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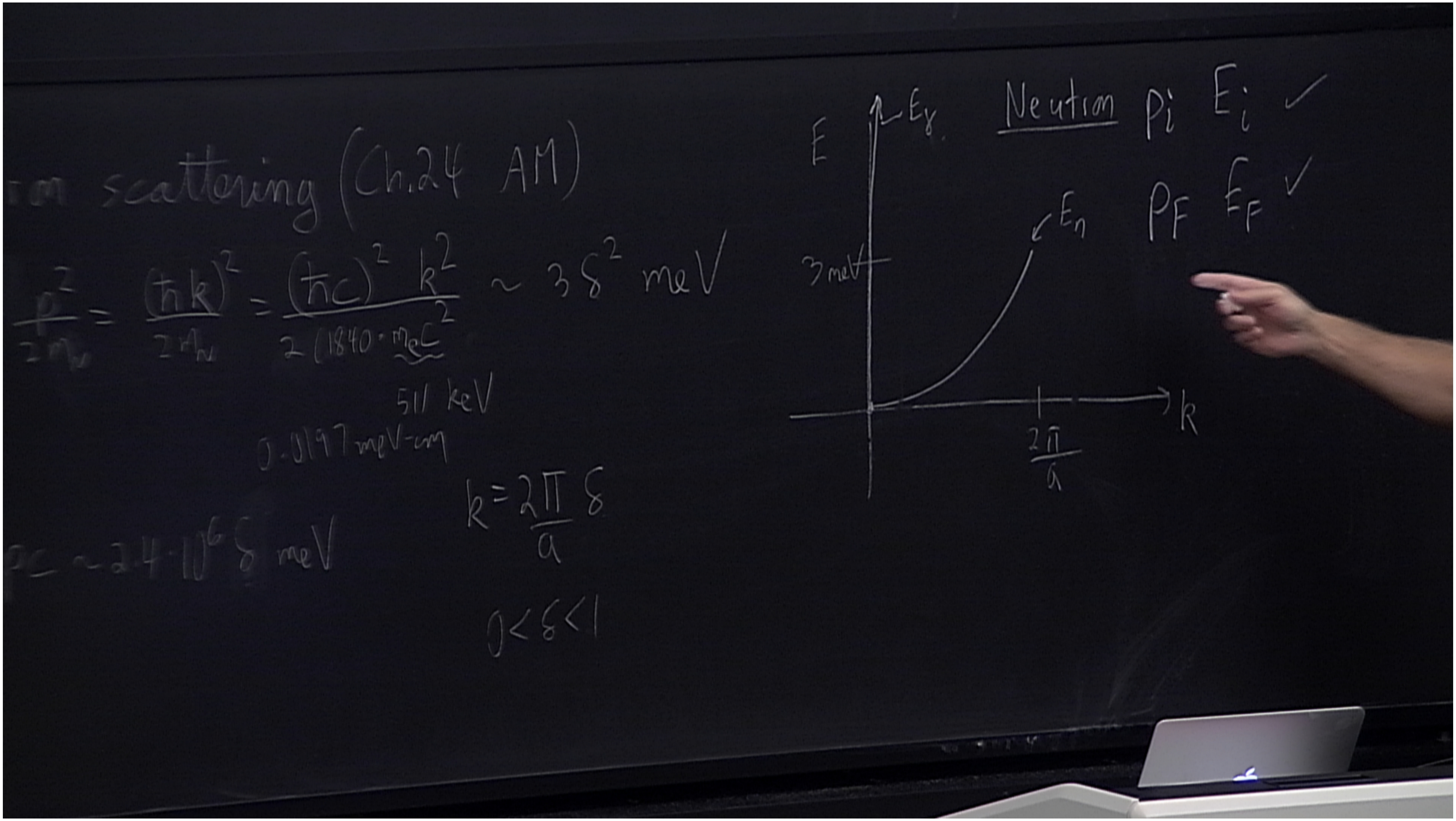
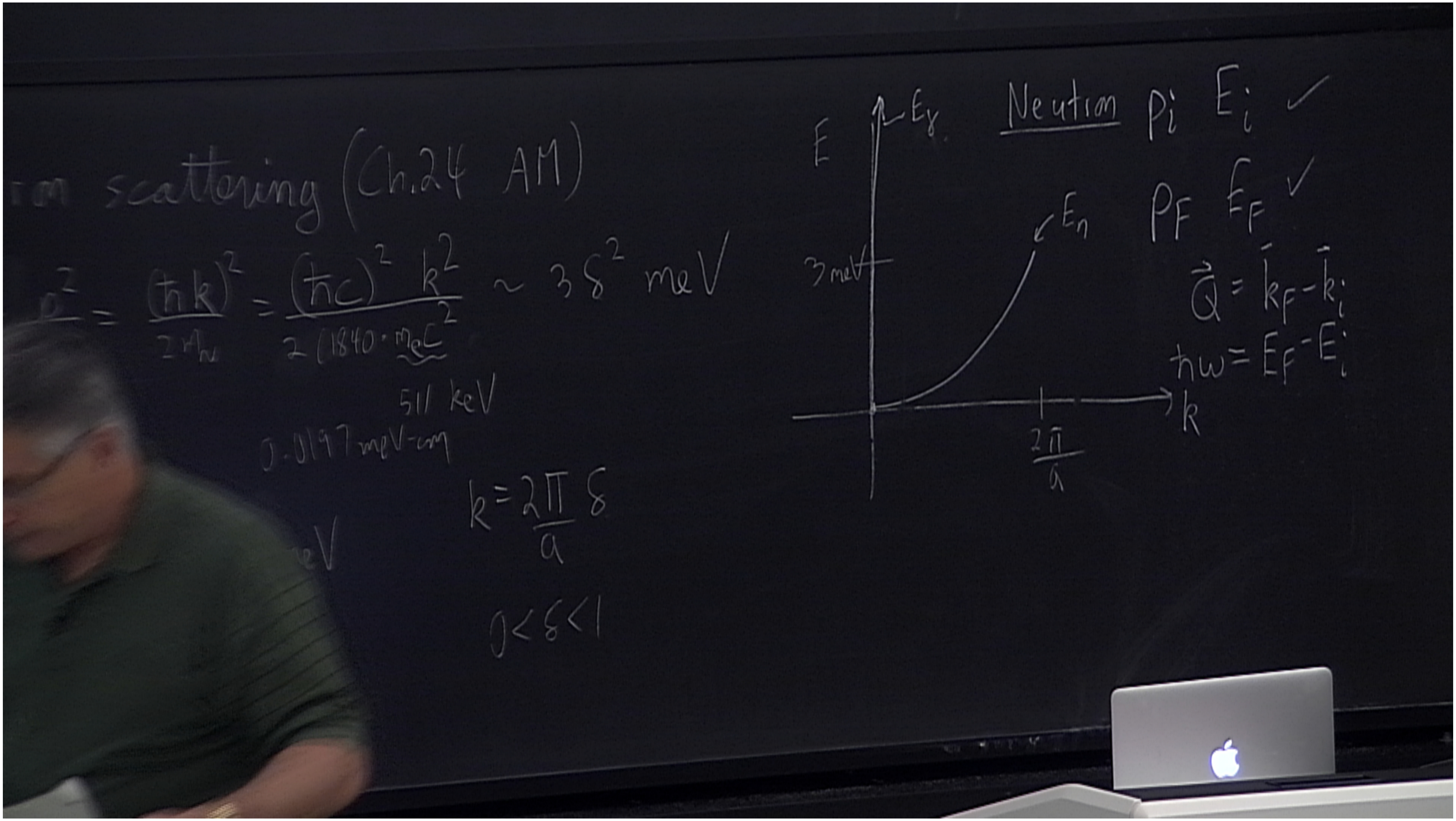
p²/2m_N = (ħk)²/2M_N = (ħc)² k² / 2(1840·m_e c²) ~ 3δ² meV
511 keV
0.0197 meV-cm
k = 2π/a δ
pc ~ 2.4·10⁶ δ meV
0 < δ < 1
E
E_γ
3 meV
E_n
k
2π/a
Neutron
p_i
E_i
p_F


scattering (Ch. 24 AM)
$\frac{p^2}{2m_N} = \frac{(\hbar k)^2}{2M_N} = \frac{(\hbar c)^2 k^2}{2(1840 \cdot m_e c^2)} \sim 38^2$ meV
511 keV
0.0197 meV-cm
$k = \frac{2\pi}{a}\delta$
$0 < \delta < 1$
$pc \sim 2.4 \cdot 10^6 \delta$ meV
E
E_γ
E_n
3 meV
$\frac{2\pi}{a}$
k
Neutron p_i E_i
p_F E_F

$S(Q,\omega)$ Dynamical Structure factor

(Fourier transform of a density-density correlation fn.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511 keV
0.0197 meV-cm
k = 2π/a δ
0 < δ < 1
E
E_γ
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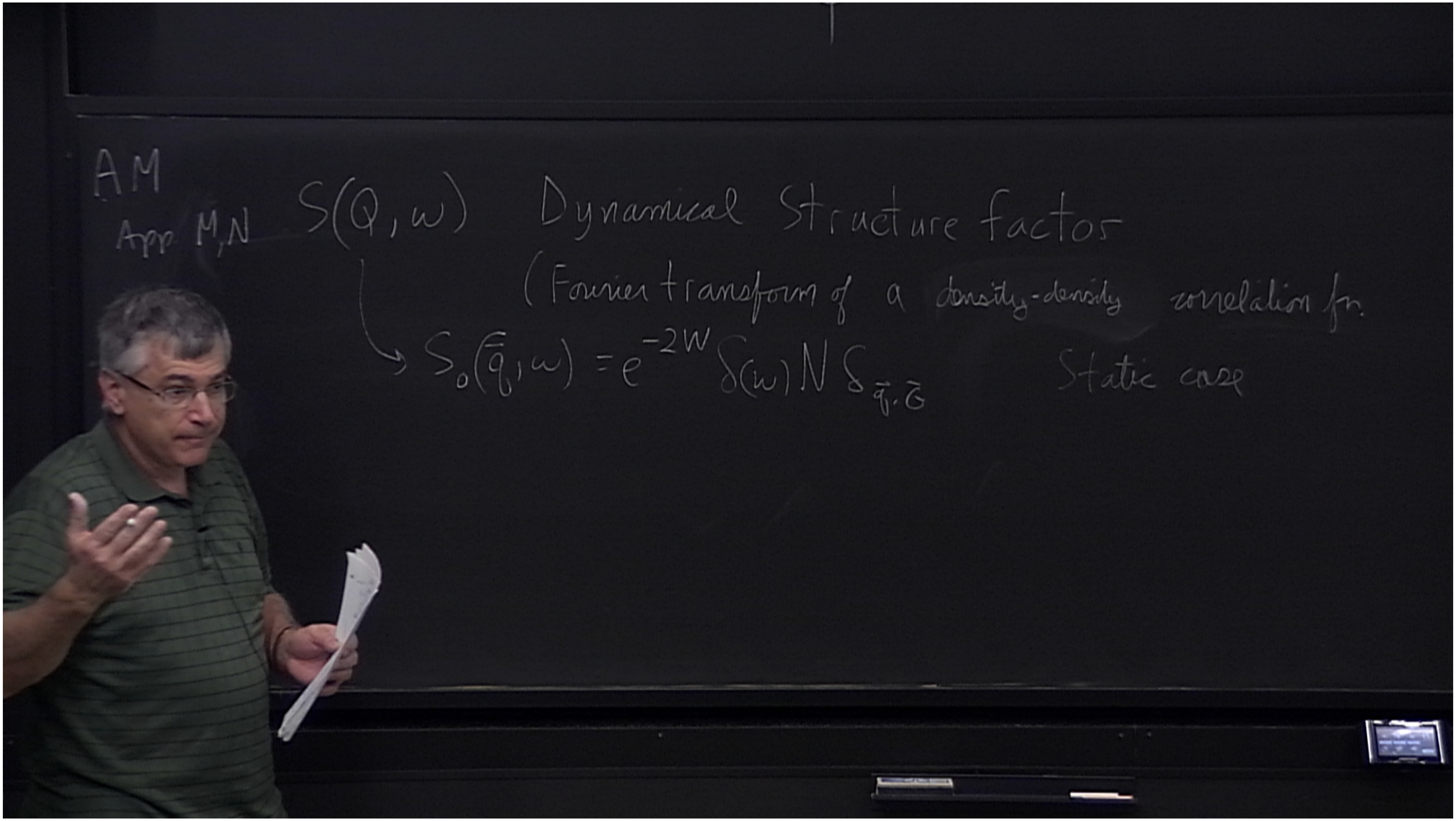
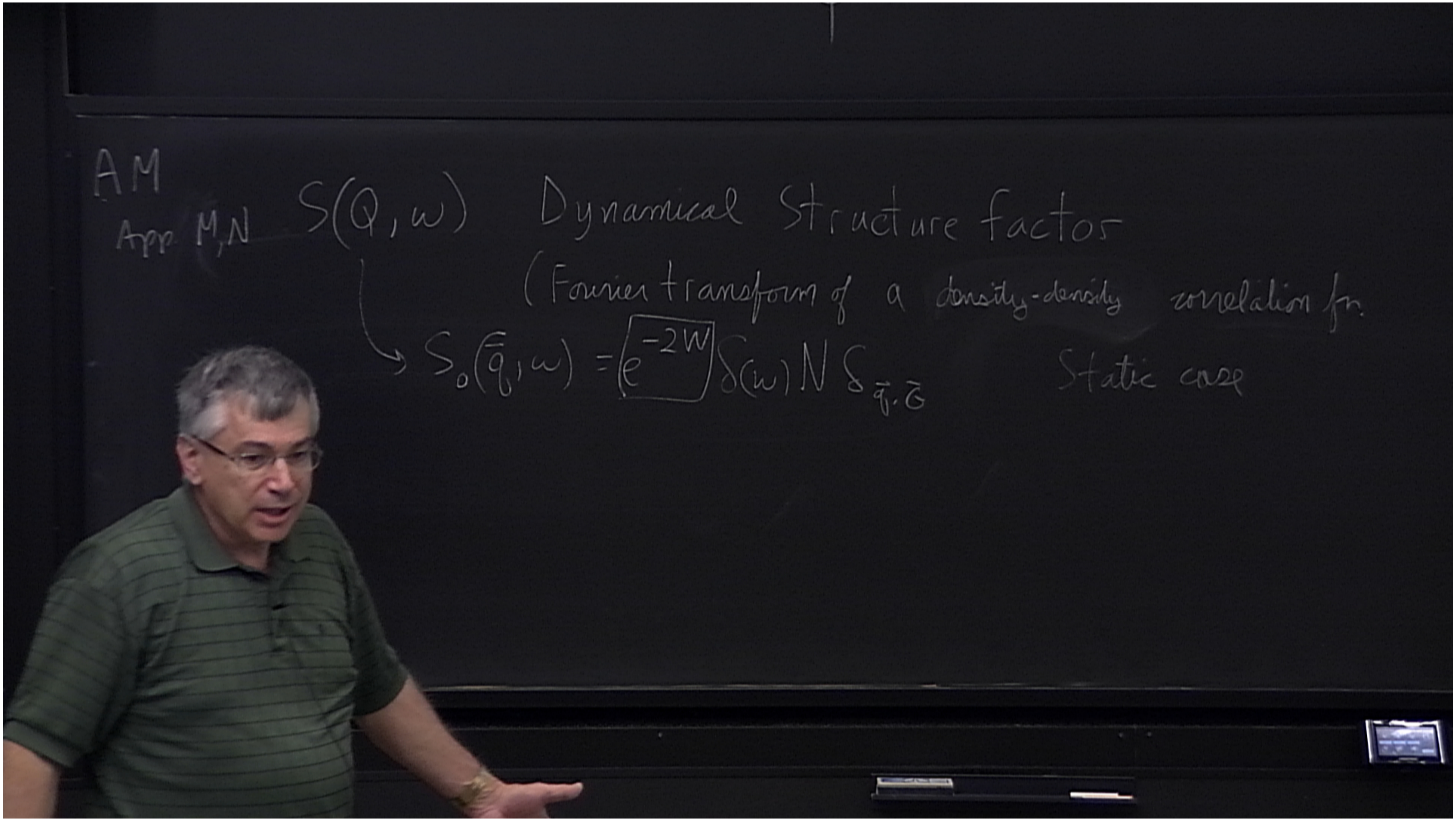
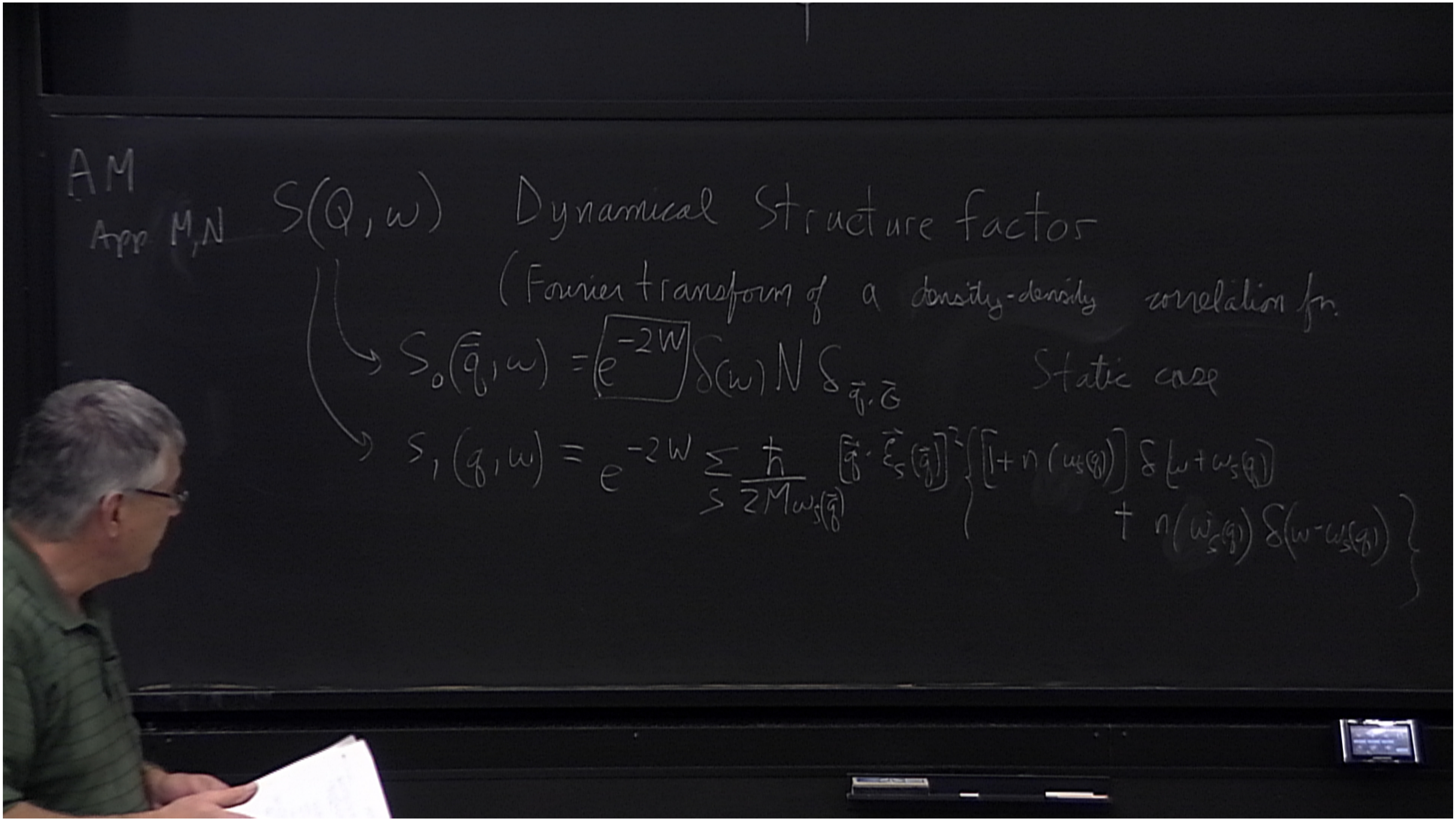
3 meV
2π/a
k
Neutron p_i E_i
p_F E_F
Q = k_F - k_i
ħω = E_F - E_i


AM
App M,N
$S(Q,\omega)$ Dynamical Structure factor
(Fourier transform of a density-density correlation fn.
$S_0(\vec{q},\omega) = e^{-2W}\delta(\omega) N \delta_{\vec{q},\vec{G}}$
Static case


AM
App. M,N
S(Q, ω) Dynamical Structure factor
(Fourier transform of a density-density correlation fn.
S0(q, ω) = e^-2W δ(ω) N δq,G
Static case



AM
App. M,N
$S(Q,\omega)$ Dynamical Structure factor
(Fourier transform of a density-density correlation fn.
$S_0(\vec{q},\omega) = \boxed{e^{-2W}}\,\delta(\omega)\, N\, \delta_{\vec{q},\vec{G}}$
Static case
$S_1(q,\omega) = e^{-2W} \sum_s \frac{\hbar}{2M\omega_s(\vec{q})} [\vec{q}\cdot\vec{\xi}_s(\vec{q})]^2 \{ [1+n(\omega_s(q))]\, \delta(\omega+\omega_s(q))$
$+\, n(\omega_s(q))\, \delta(\omega-\omega_s(q)) \}$

Brockhouse et al. PR 128, 1099 (1962)

Pb

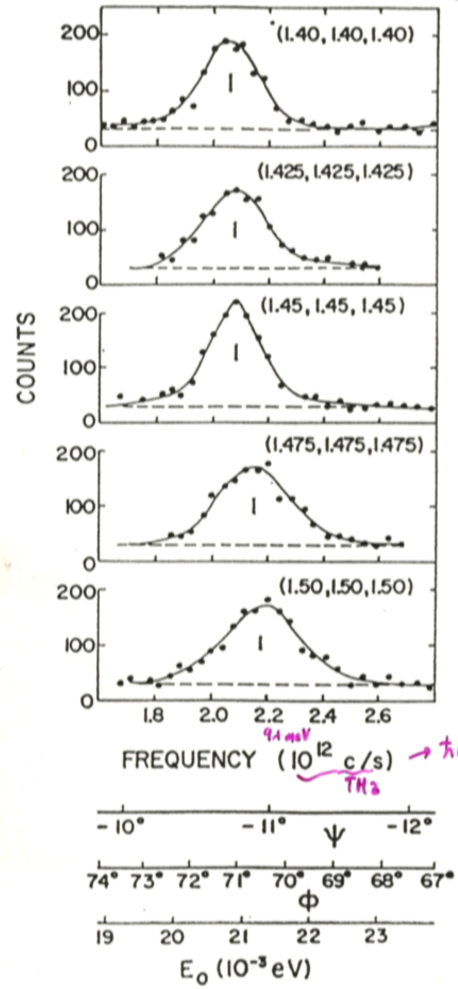


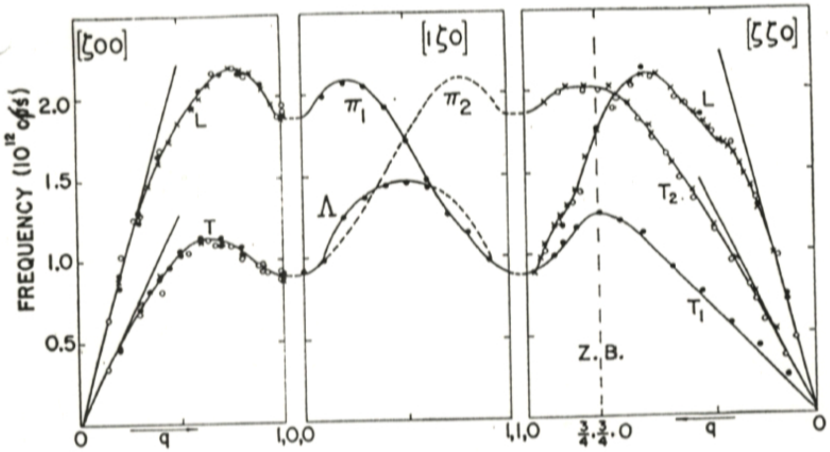
Fig. 4. A set of "constant **Q**" experiments made at points between (1.4,1.4,1.4) and (1.5,1.5,1.5) in reciprocal space. Auxiliary scales for the three experimental variables E_0, ϕ, and ψ are shown at the bottom for the (1.5,1.5,1.5) experiment, also shown in Fig. 3.

$\rightarrow \hbar\omega = h\nu = 4.136 \cdot 10^{-12}$ meV

$E_n' < E_0$

Final

initial



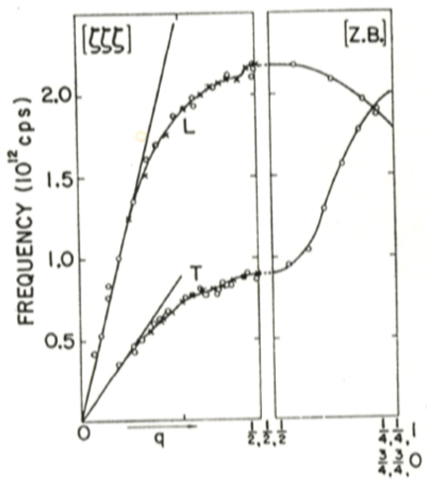


FIG. 5. The dispersion curves for lead at 100°K, plotted so as to show the inter-relation of the various branches. The older measurements (reference 2) are shown by open and closed circles, the most recent by crosses. The straight lines through the origin give the initial slopes of the curves as calculated from the elastic constants (Table III).

Pb

Brockhouse et al.

Brockhouse et al. PR 128, 1099 (1962)

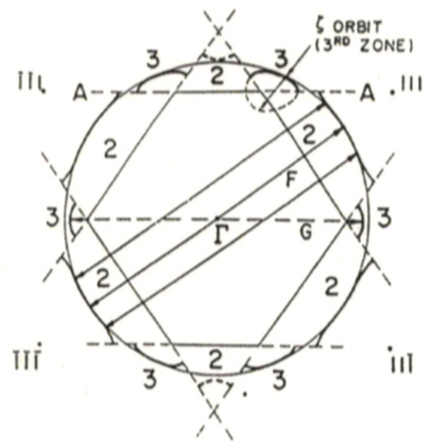


FIG. 10. Possible section through the Fermi surface of lead in a (1$\bar{1}$0) plane through the origin. The section of the free electron sphere containing four electrons is shown as a light circular line. Bragg reflection occurs where this circle intersects the reflecting planes shown, and the Fermi surface is distorted somewhat as shown. Electron scattering vectors which produce a Kohn anomaly in the [ζζζ] *L* branch are indicated by the bold double headed arrows, *F*, and in the [ζζ0] *L* branch by the dashed double headed arrow, *G*.

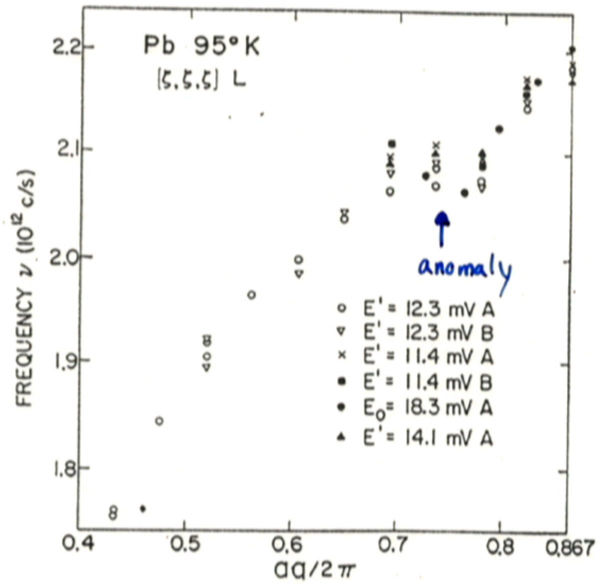


FIG. 11. Collected results for the [ζζζ] *L* branch. The letters *A* and *B* refer to zones about the (1,1,1) and (2,2,2) reciprocal lattice points.

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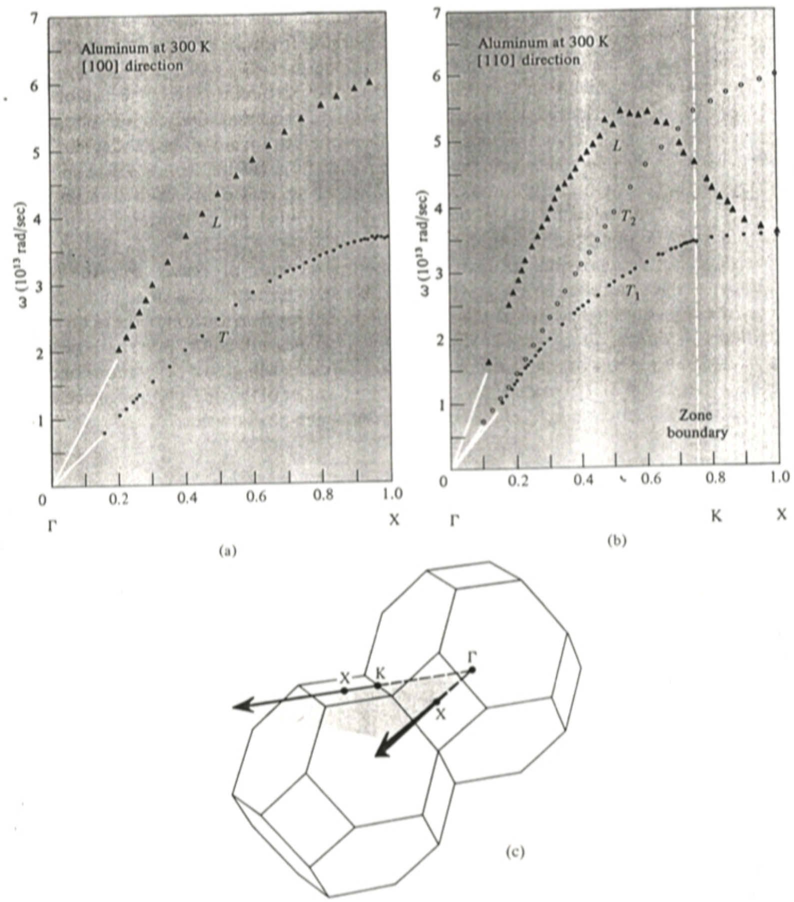

Figure 24.2
Phonon dispersion relations in aluminum, measured along the k-space lines ΓX and ΓKX by neutron scattering. The estimated error in frequency is 1 to 2 percent. Each point represents an observed neutron group. (After J. Yarnell et al., *Lattice Dynamics*, R. F. Wallis, ed., Pergamon, New York, 1965.) Note that the two transverse branches are degenerate along ΓX (4-fold axis), but not along ΓK (2-fold axis). See Chapter 22.