Title: PSI 2016/2017 Condensed Matter - Lecture 2

Date: Nov 08, 2016 10:45 AM

URL: http://pirsa.org/16110053

Abstract:

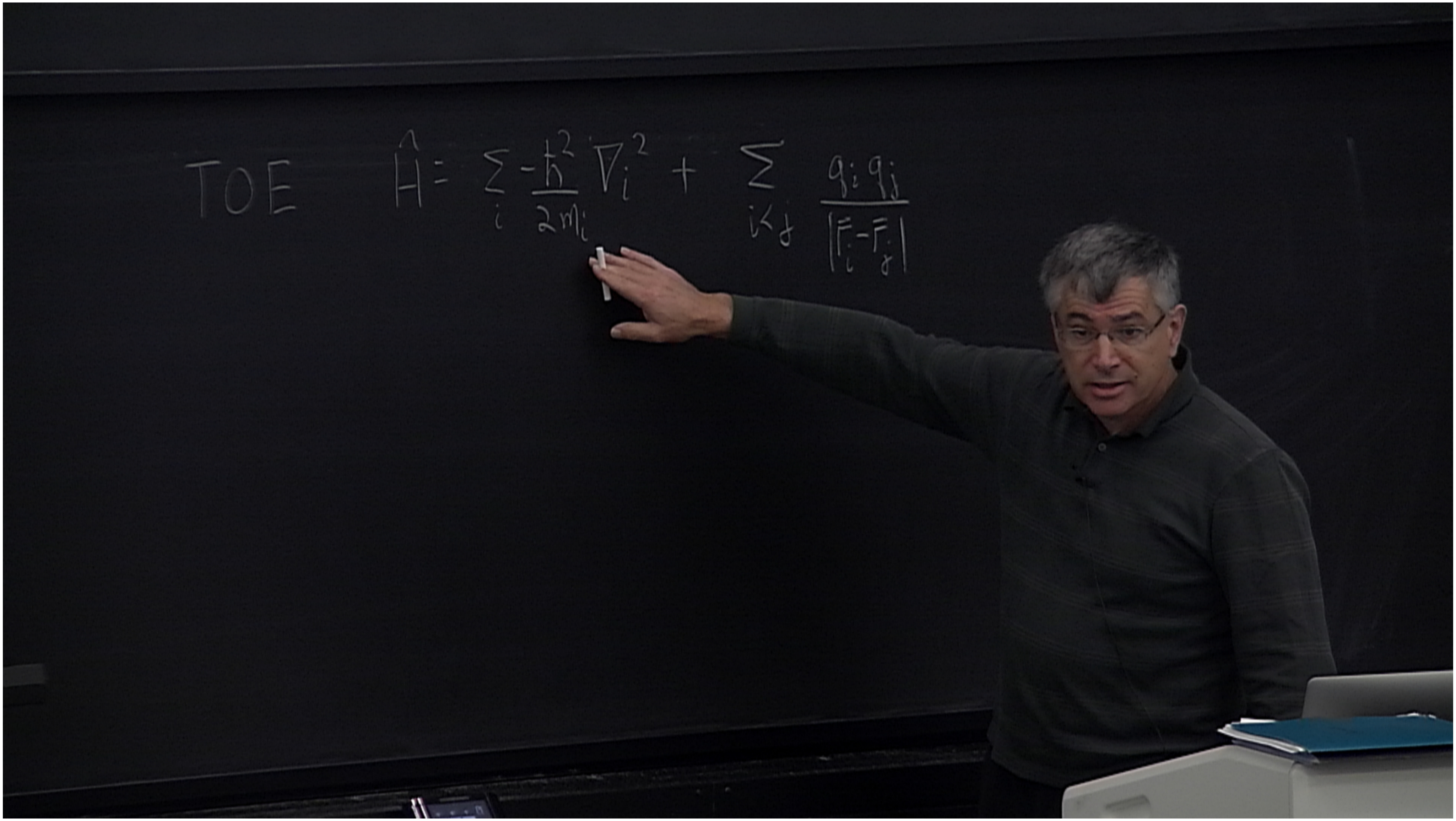
Perimeter: Condensed Matter Fall 2016

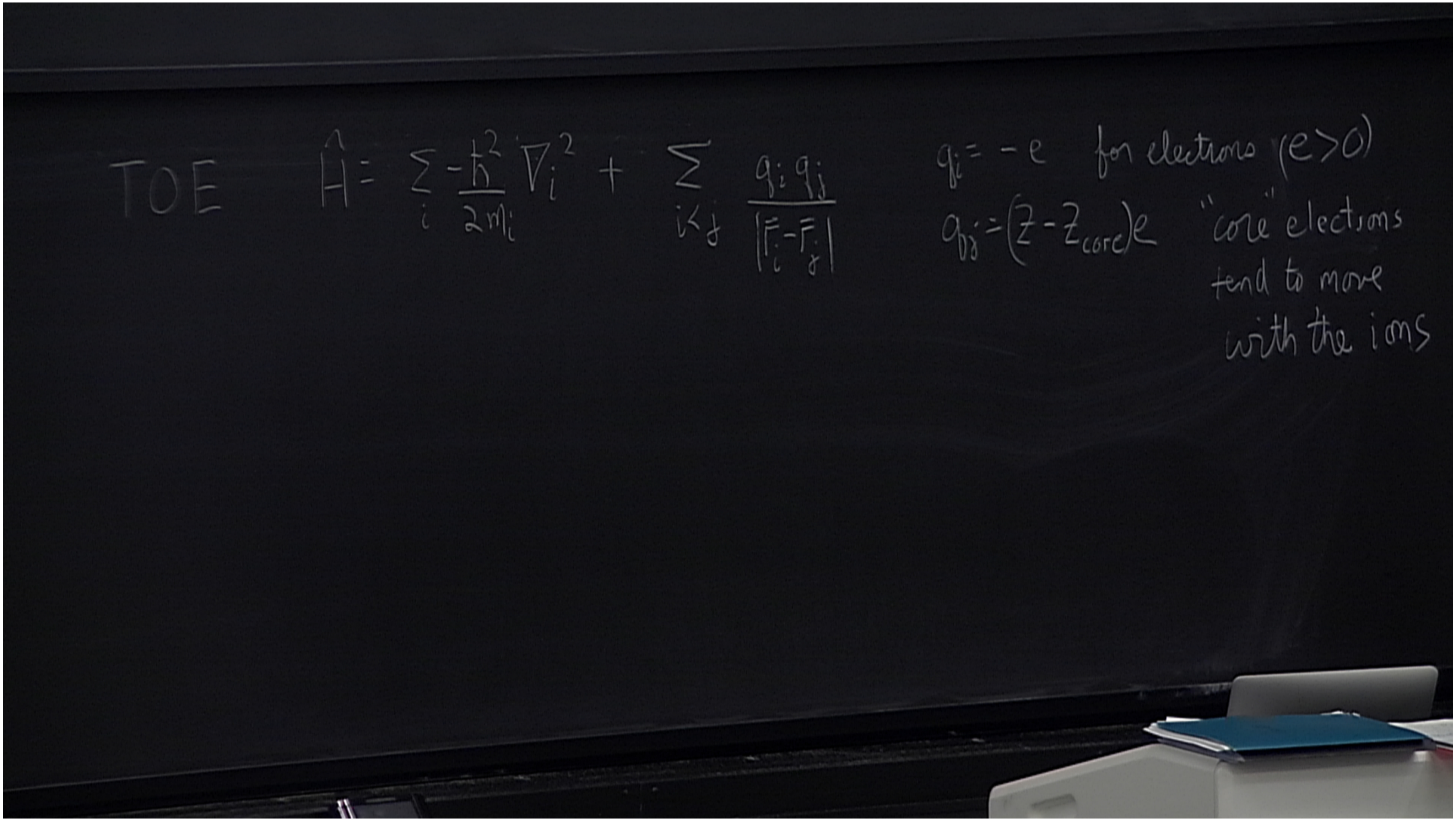
…Metals, Insulators, Magnets, and Superconductors…

supplementary material to Lecture 2, etc.

F. Marsiglio

fm3@ualberta.ca


TOE
$\hat{H} = \sum_i -\frac{\hbar^2}{2m_i}\nabla_i^2 + \sum_{i<j} \frac{q_i q_j}{|\vec{r}_i - \vec{r}_j|}$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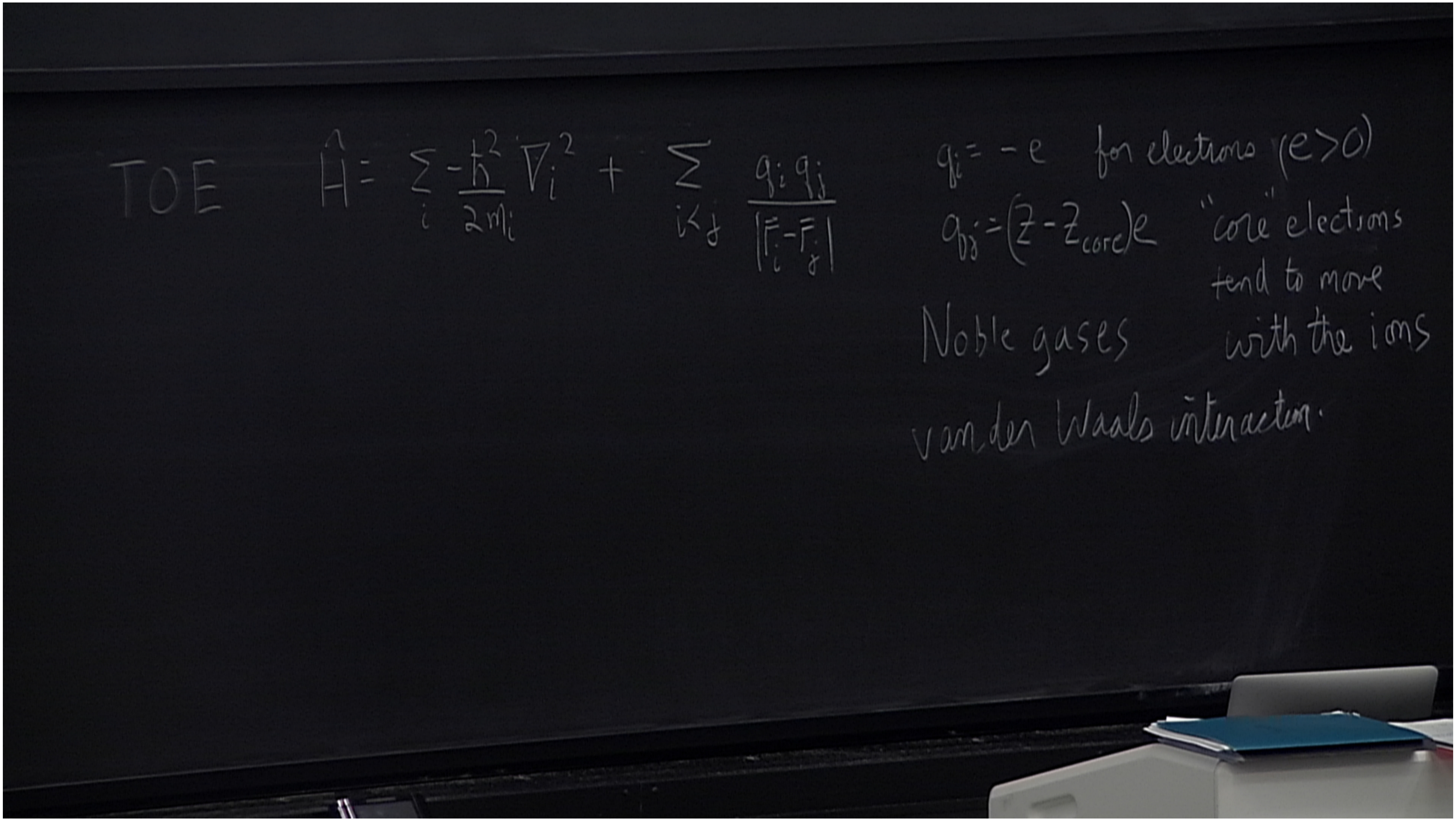
$q_i = -e$ for electrons $(e>0)$
$q_\gamma = (Z - Z_{core})e$
"core" electrons tend to move with the ions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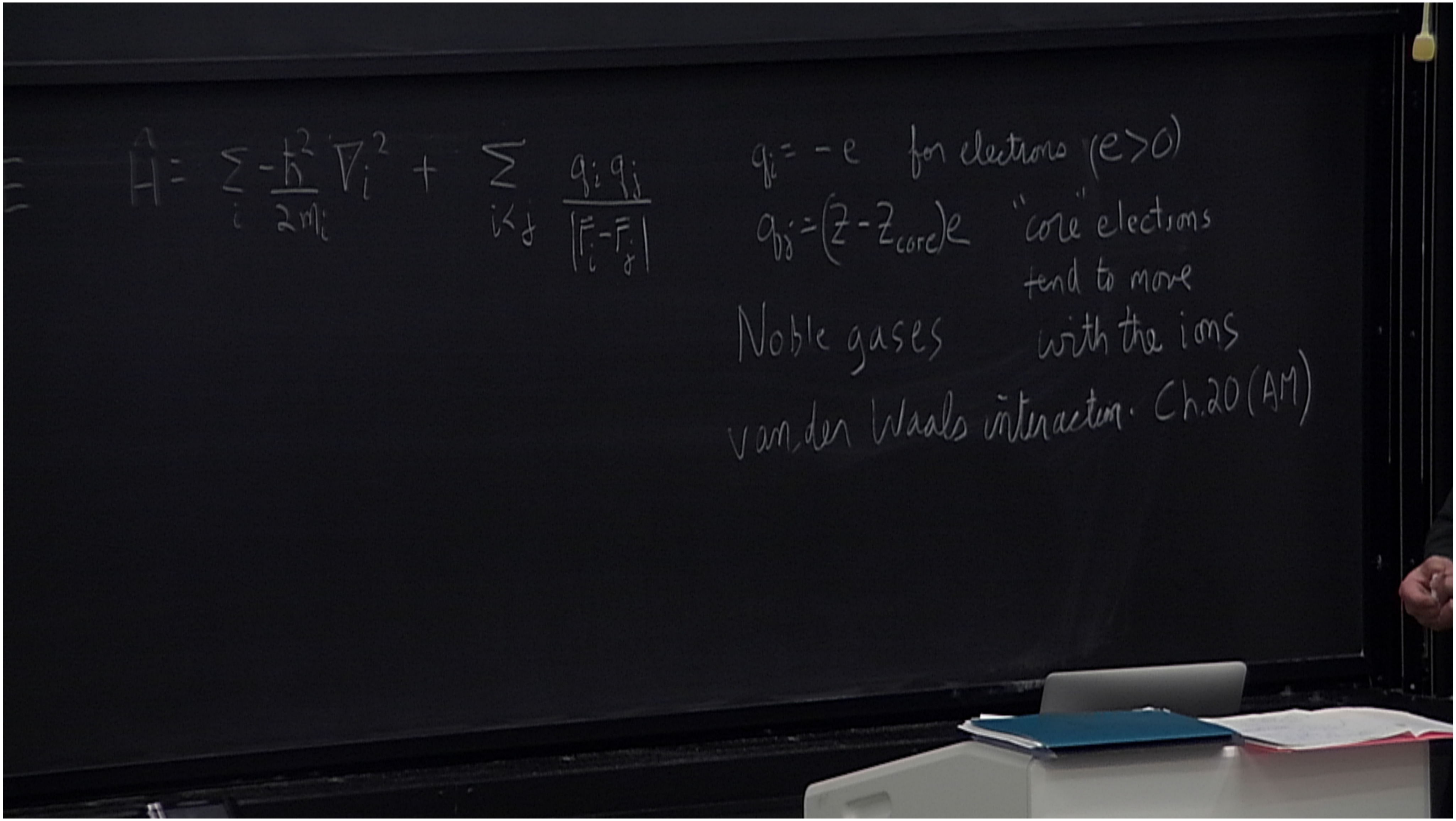
Noble gases
van der Waals interaction.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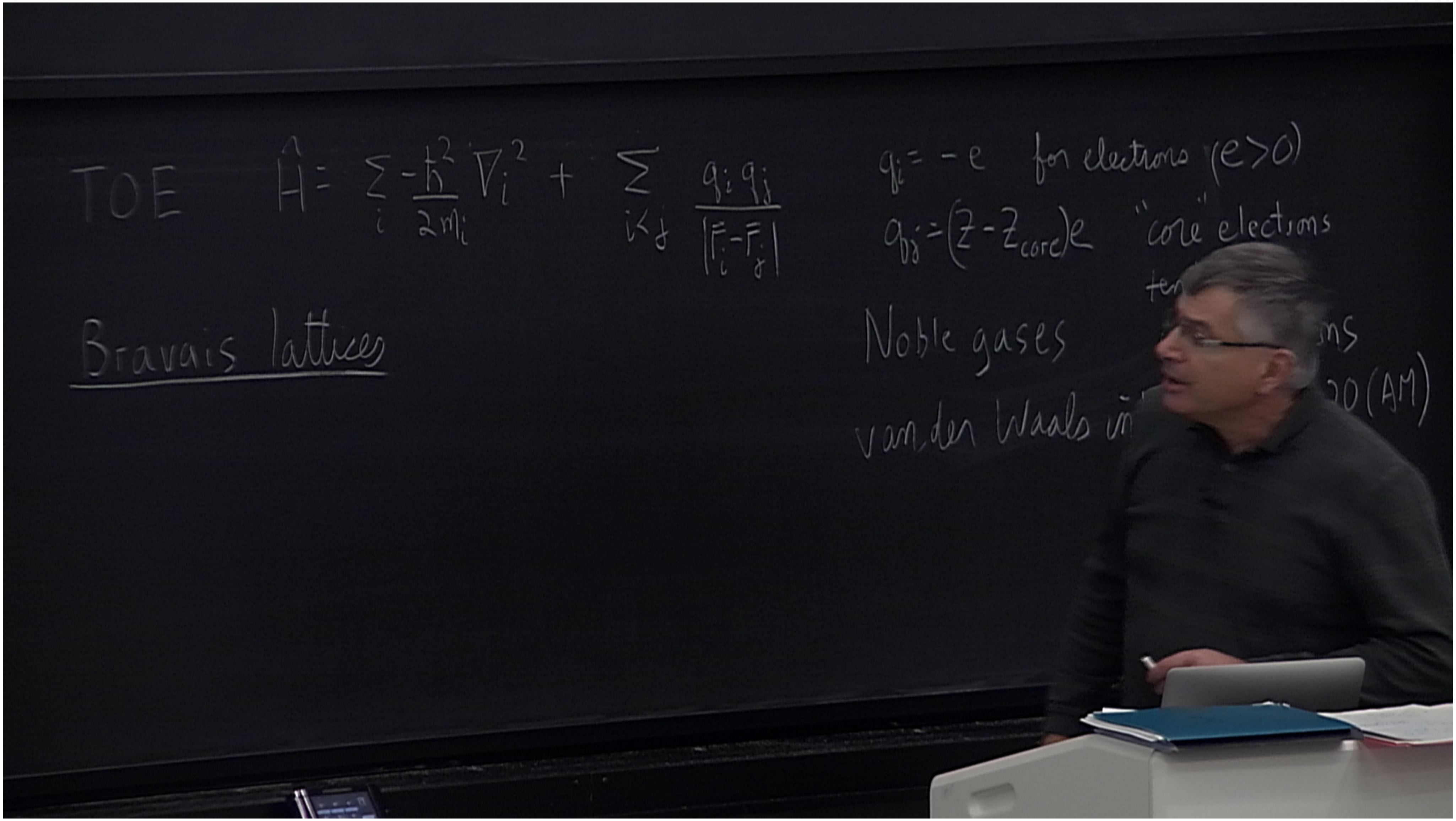
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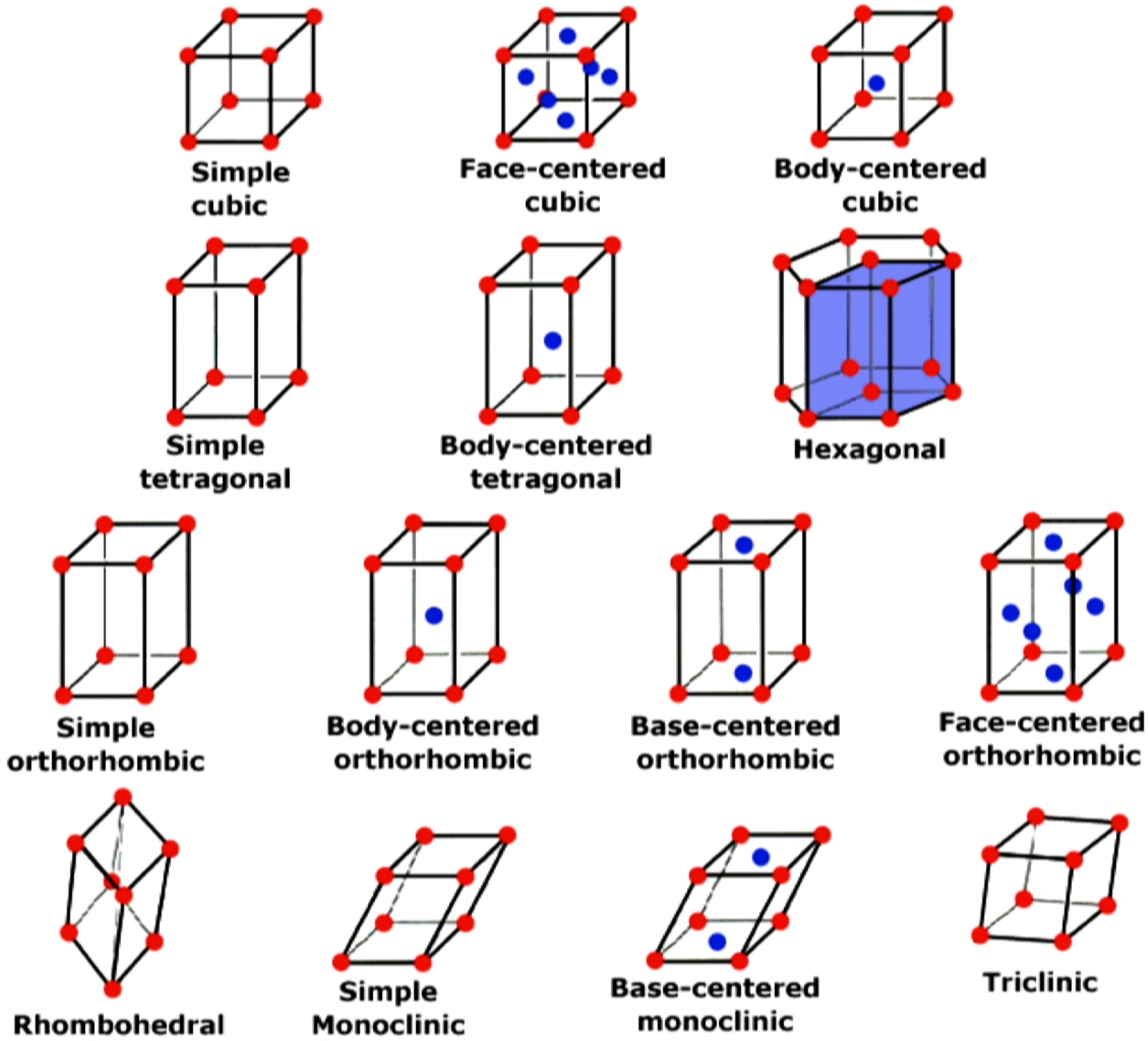
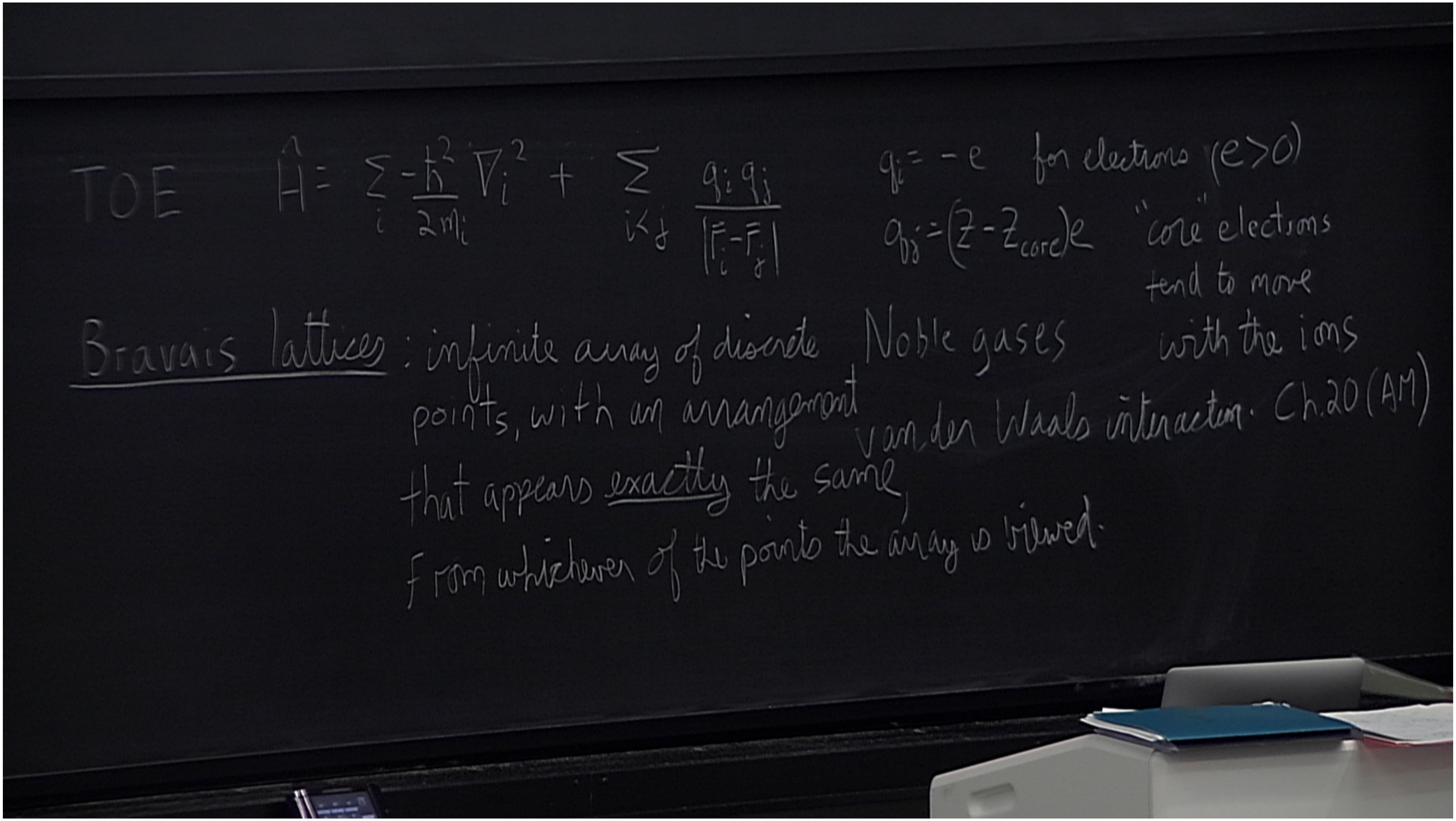
Bravais lattices
Noble gases
van der Waals



http://www.seas.upenn.edu/~chem101/sschem/solidstatechem.html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Noble gases
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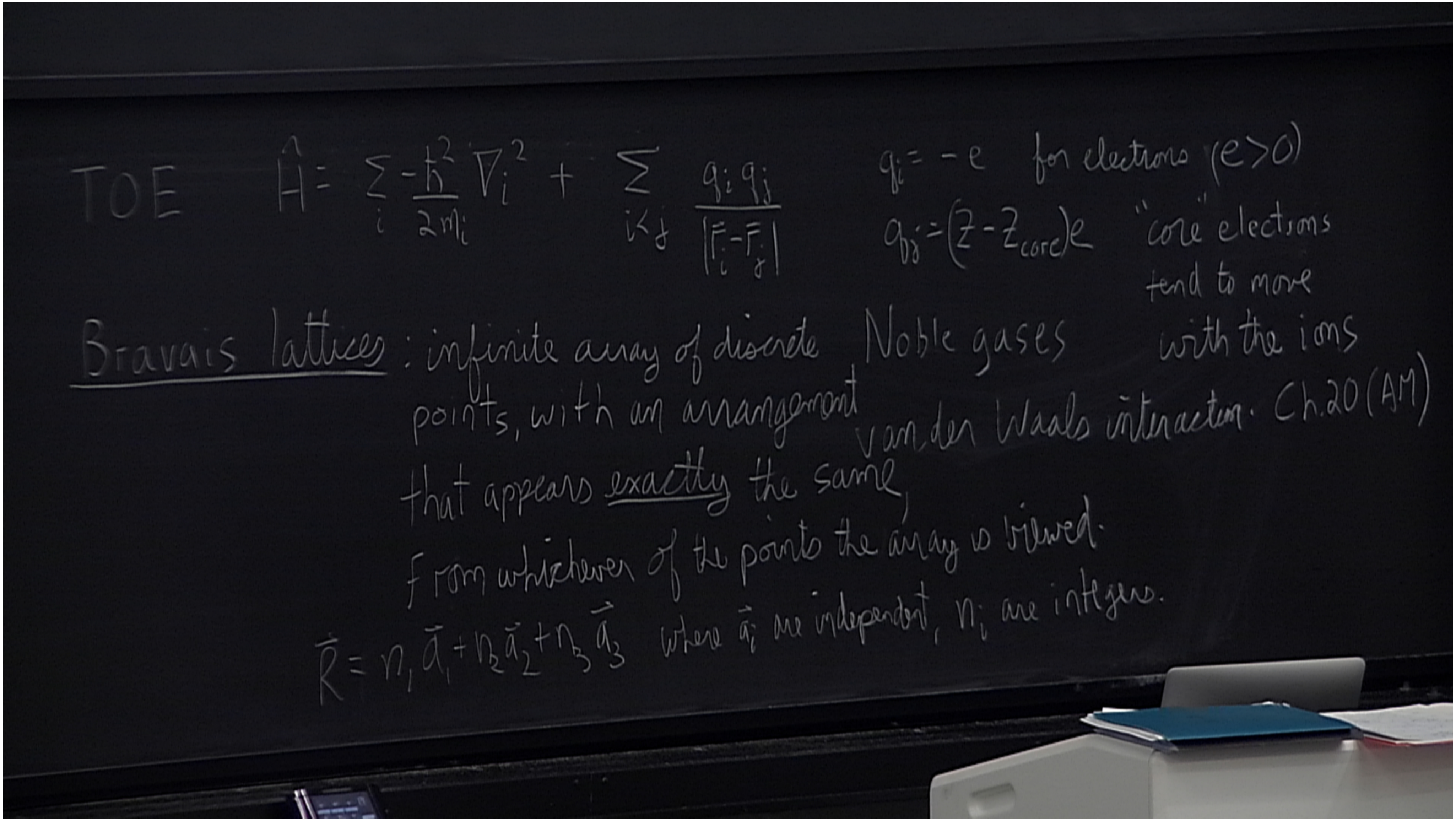
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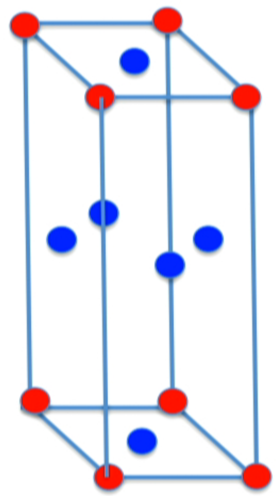
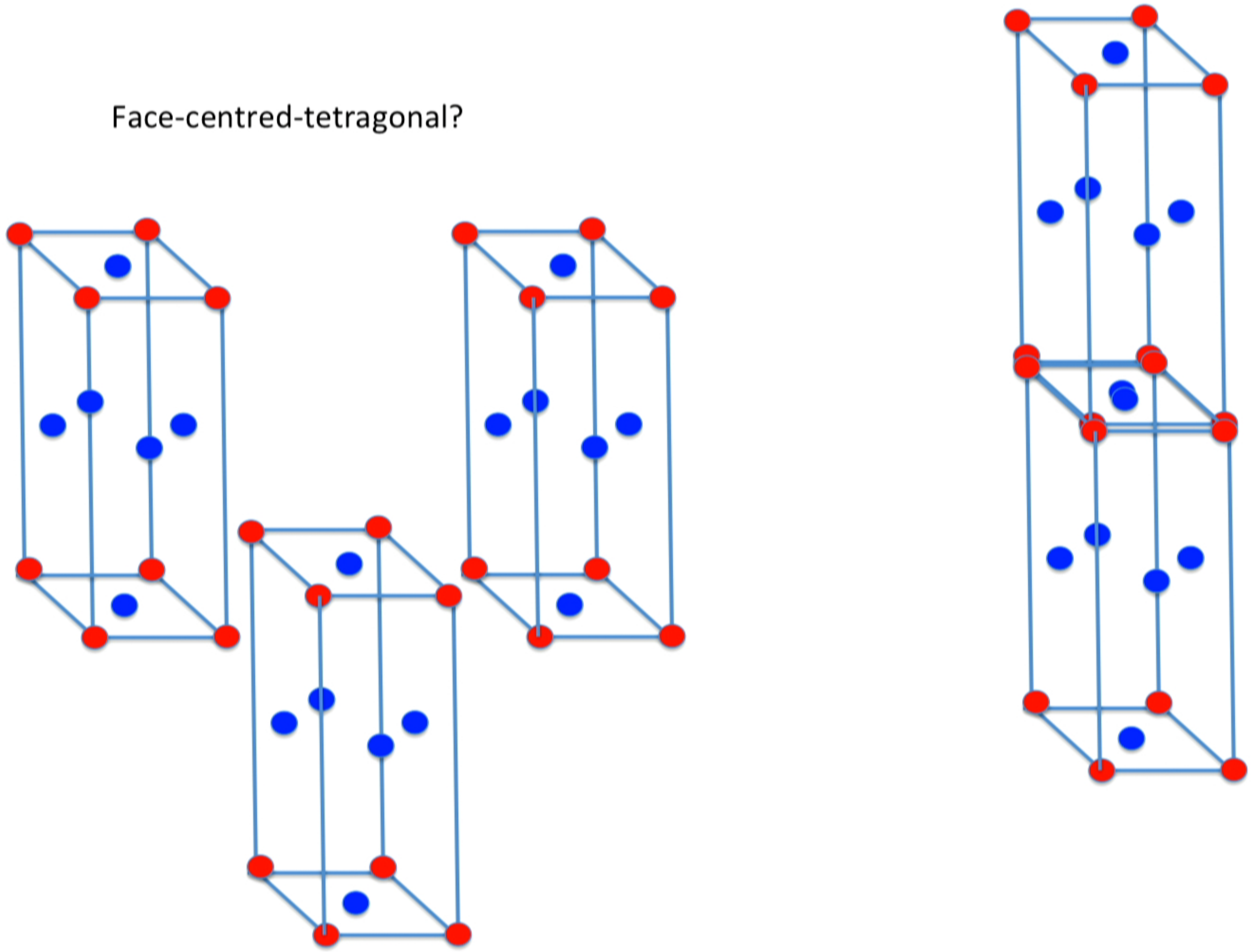
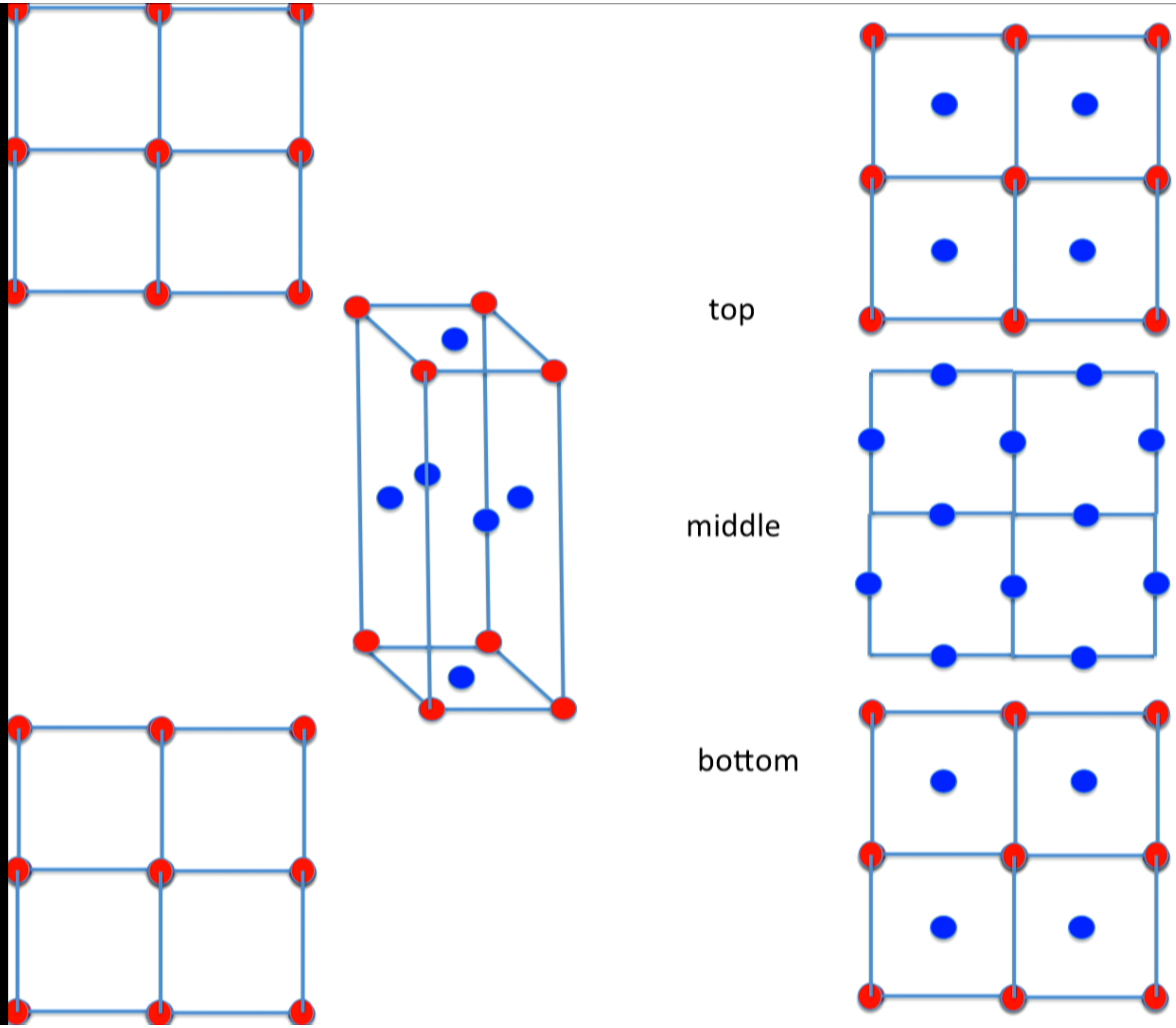
Noble gases
van der Waals interaction. Ch.20 (AM)
$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$ where $\vec{a}_i$ are independent, n_i are integers.

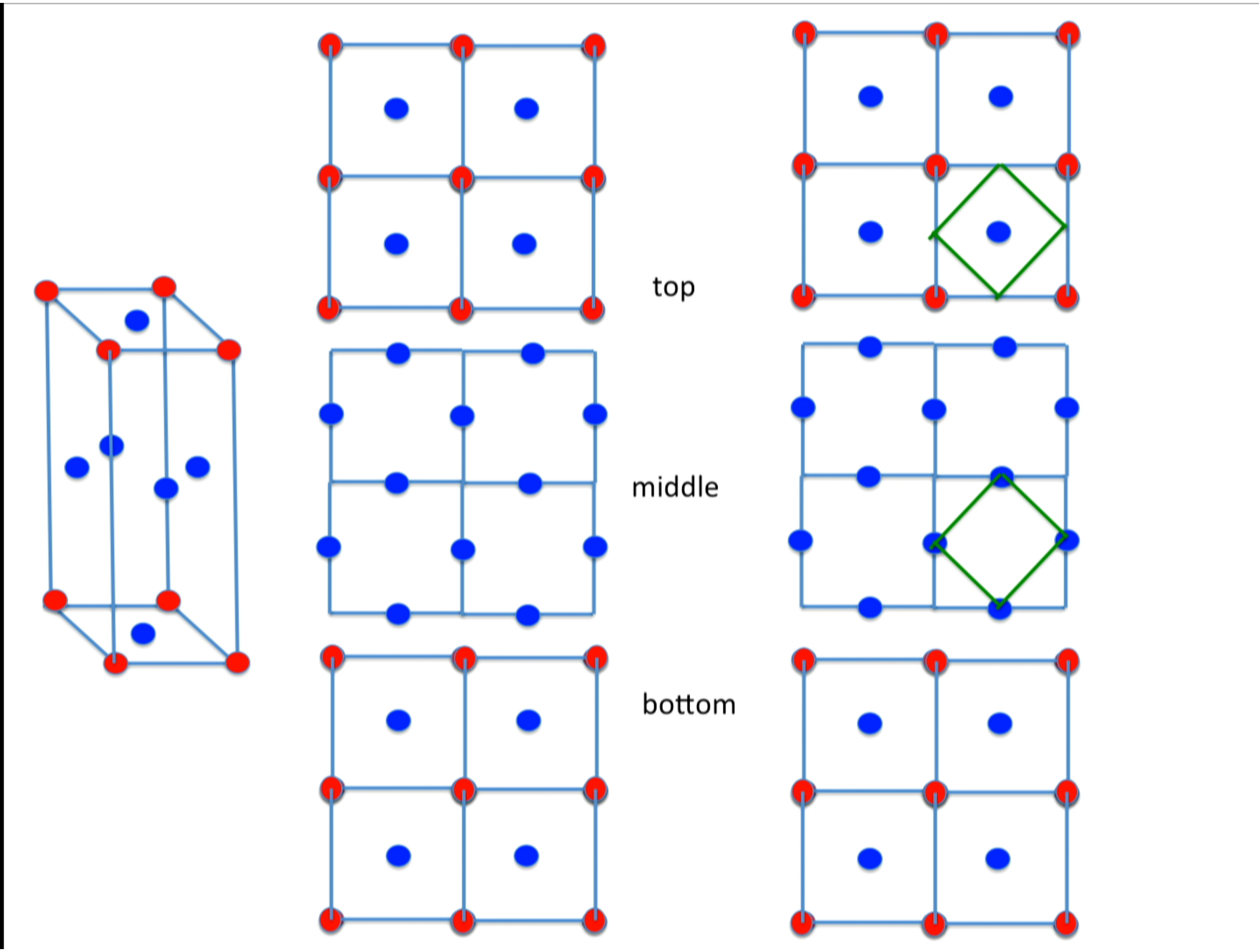
Face-centred-tetragonal?



Face-centred-tetragonal?




top
middle
bottom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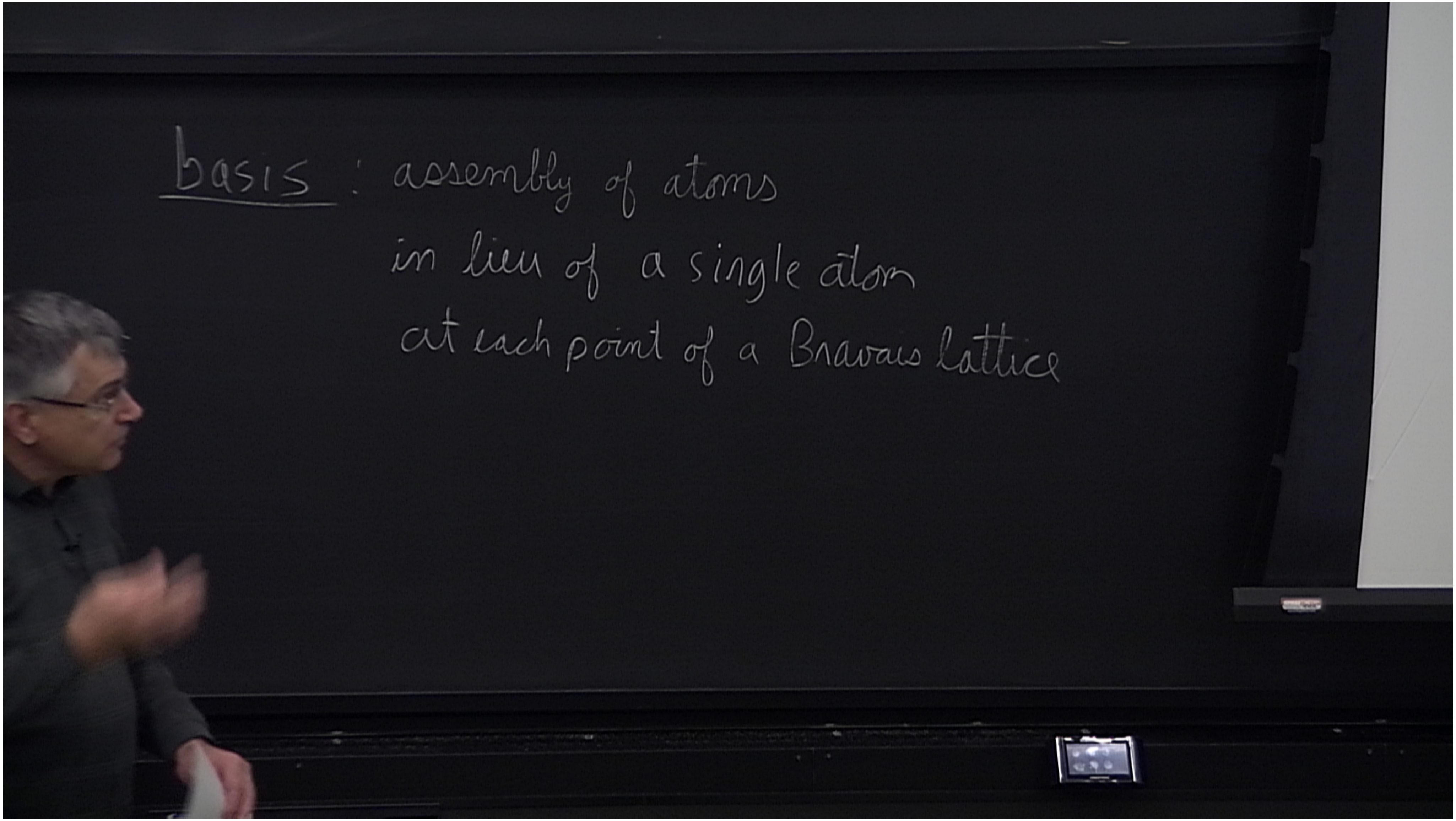
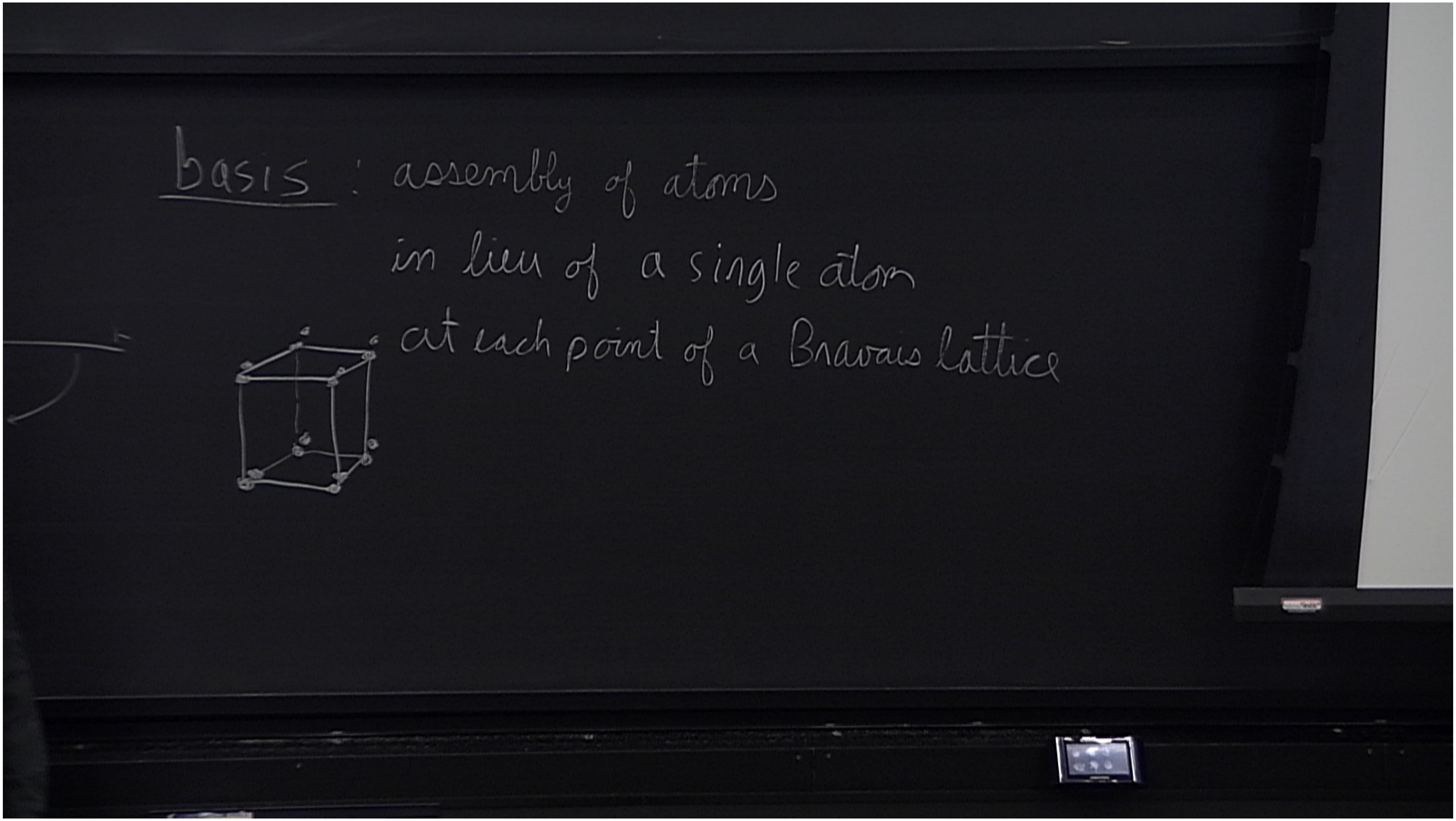

basis: assembly of atoms
in lieu of a single atom
at each point of a Bravais lattice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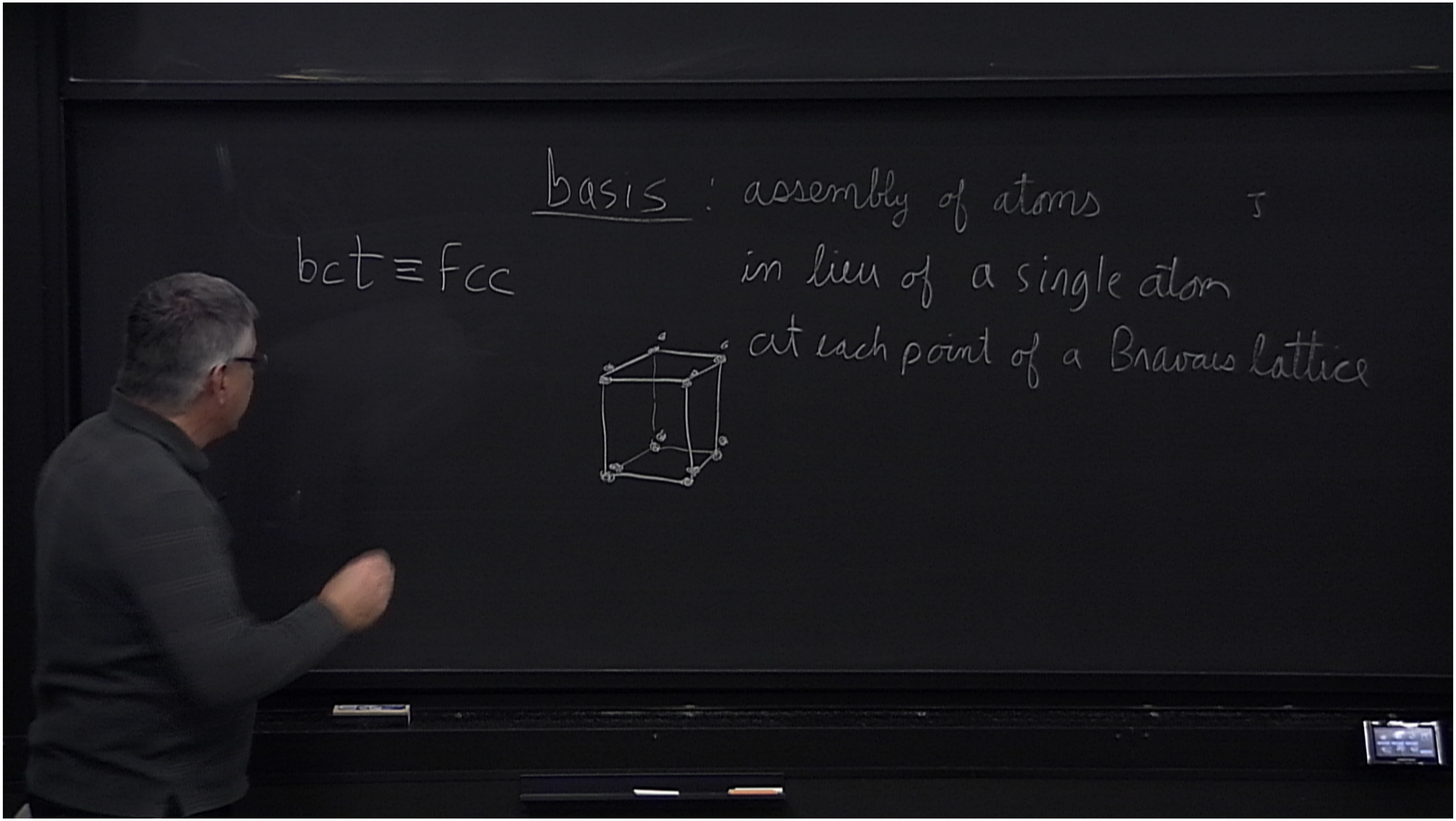
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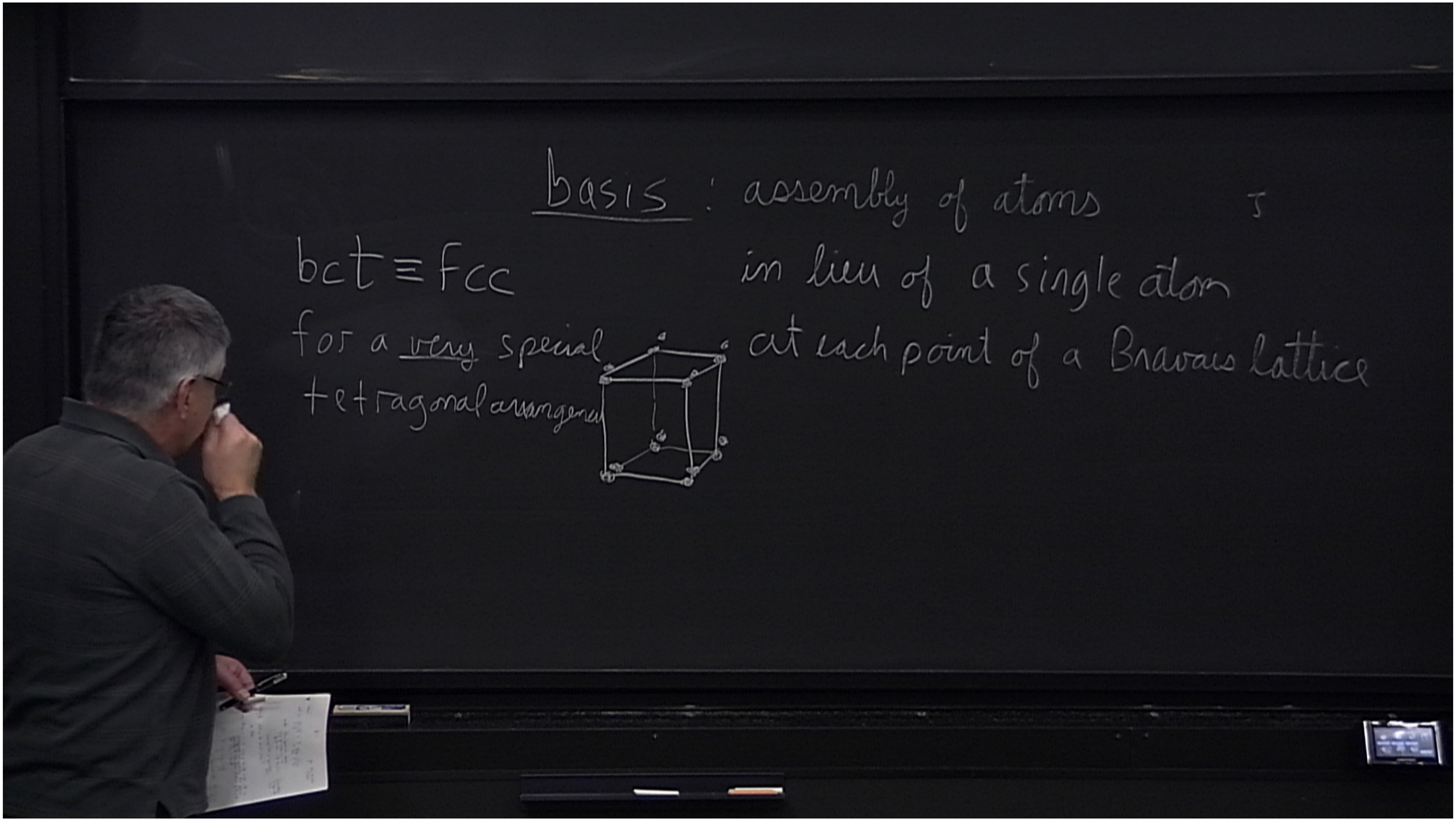
bct ≡ fcc


basis : assembly of atoms
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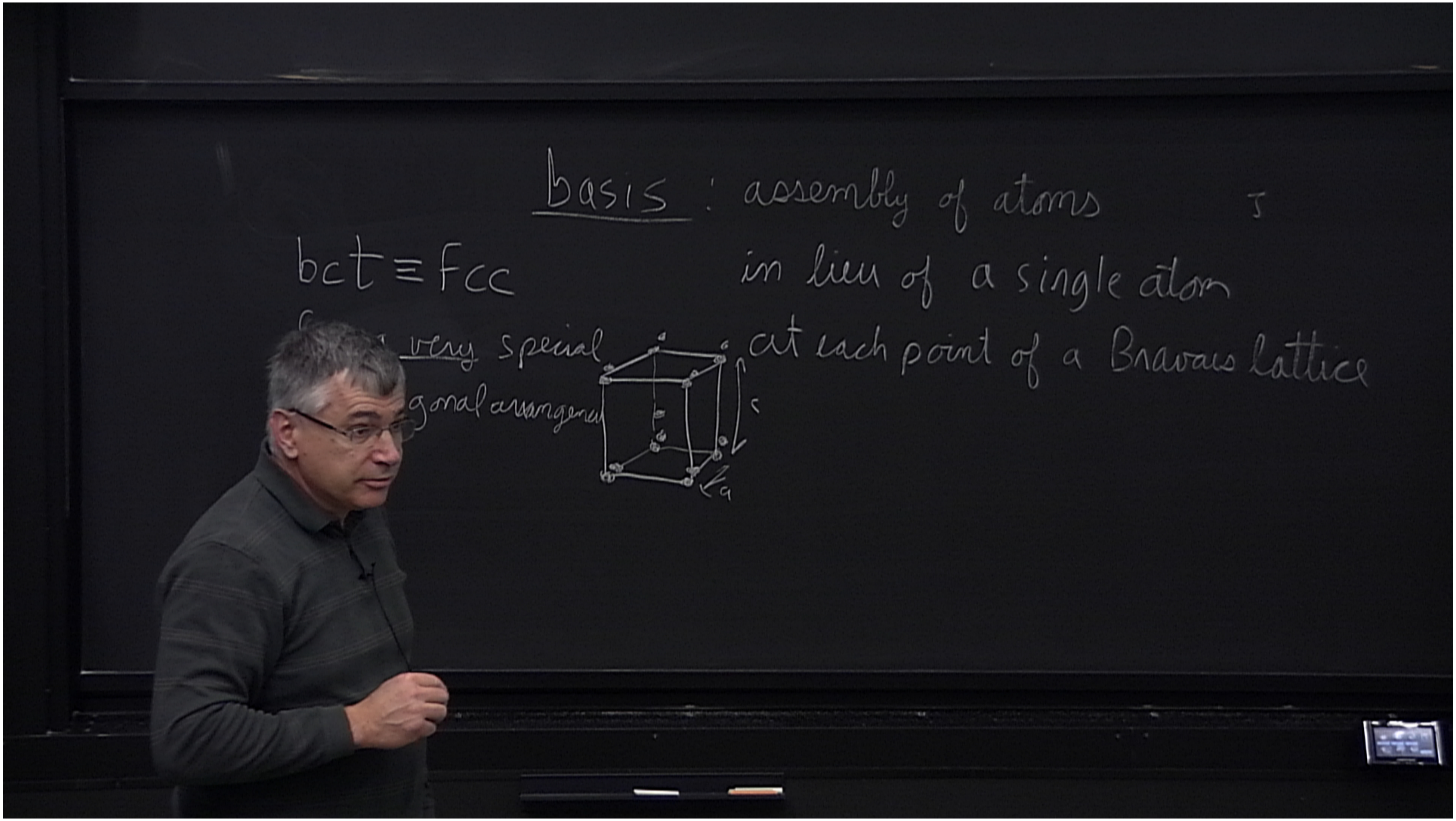
bct ≡ fcc
for a very special
tetragonal arrangement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very special
at each point of a Bravais lattice
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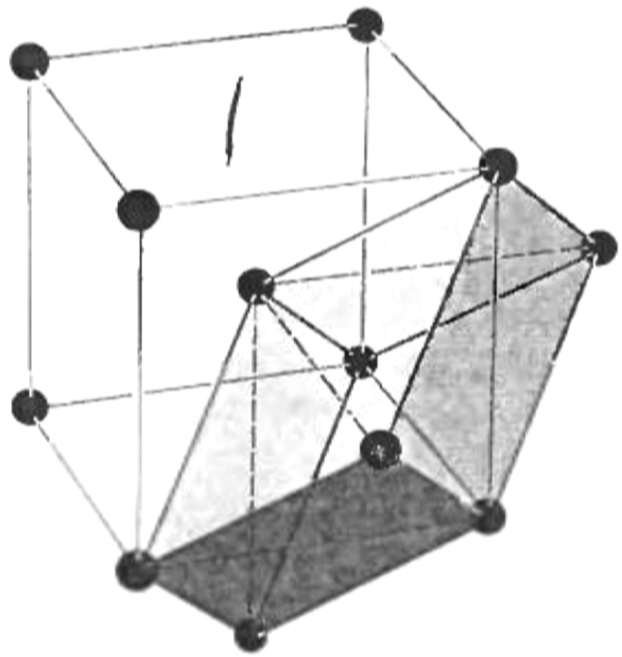
Body-centered cubic (BCC)



- Primitive translation vectors

$$\vec{a}' = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$

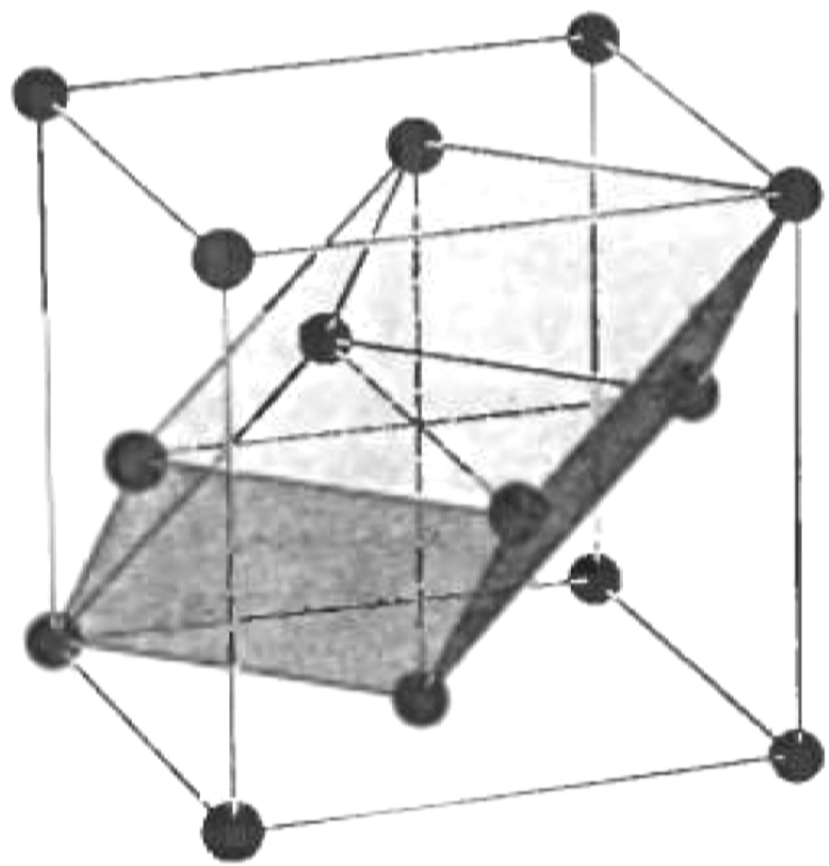
$$\vec{b}' = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z})$$

$$\vec{c}' = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z})$$

orthogonal vectors of unit length

Aschroft and Mermin, p. 73

Face-centered cubic (FCC)



- Primitive translation vectors

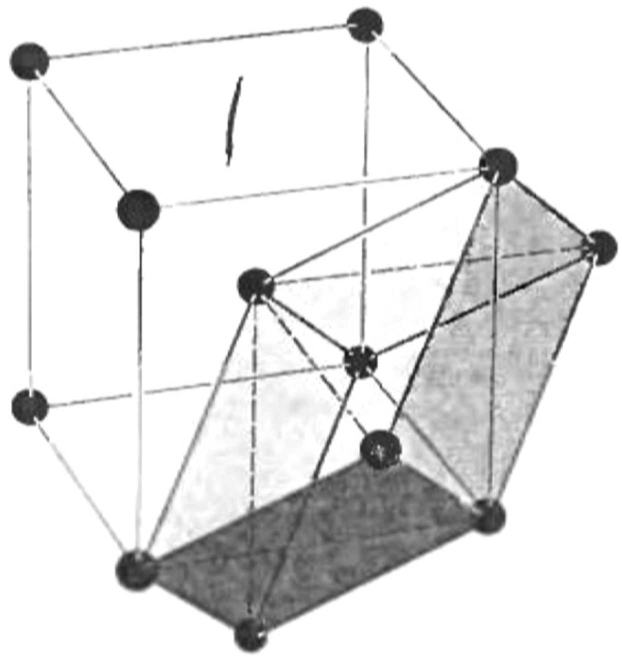
$$\vec{a}' = \frac{a}{2}(\hat{x} + \hat{y});$$

$$\vec{b}' = \frac{a}{2}(\hat{y} + \hat{z})$$

$$\vec{c}' = \frac{a}{2}(\hat{z} + \hat{x}).$$

Aschroft and Mermin, p. 72

Body-centered cubic (BCC)



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Aschroft and Mermin, p. 73

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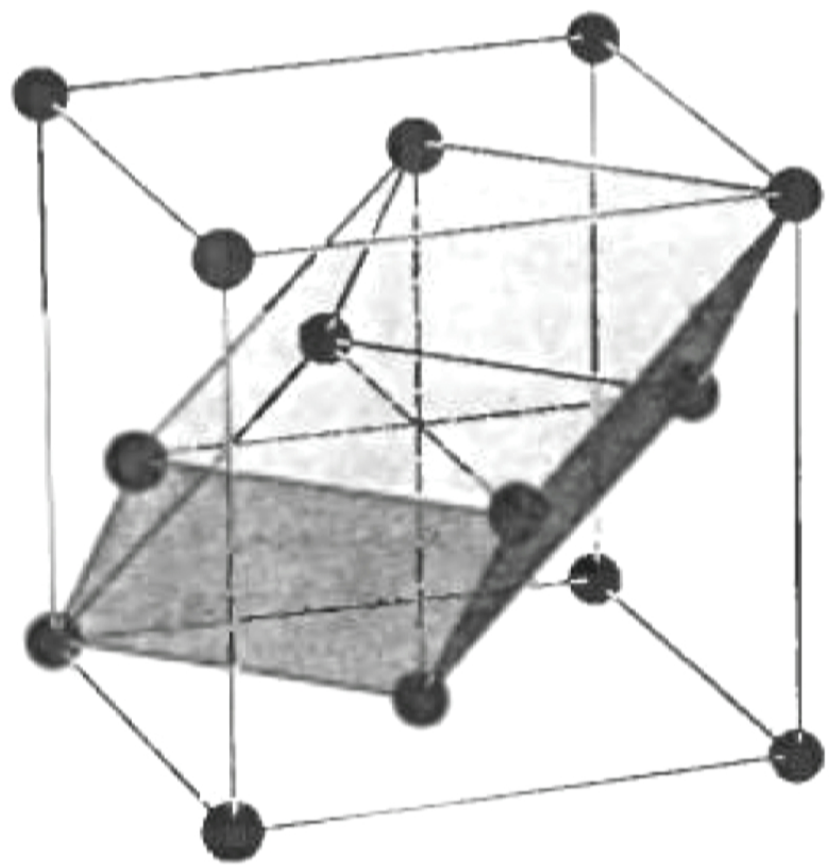

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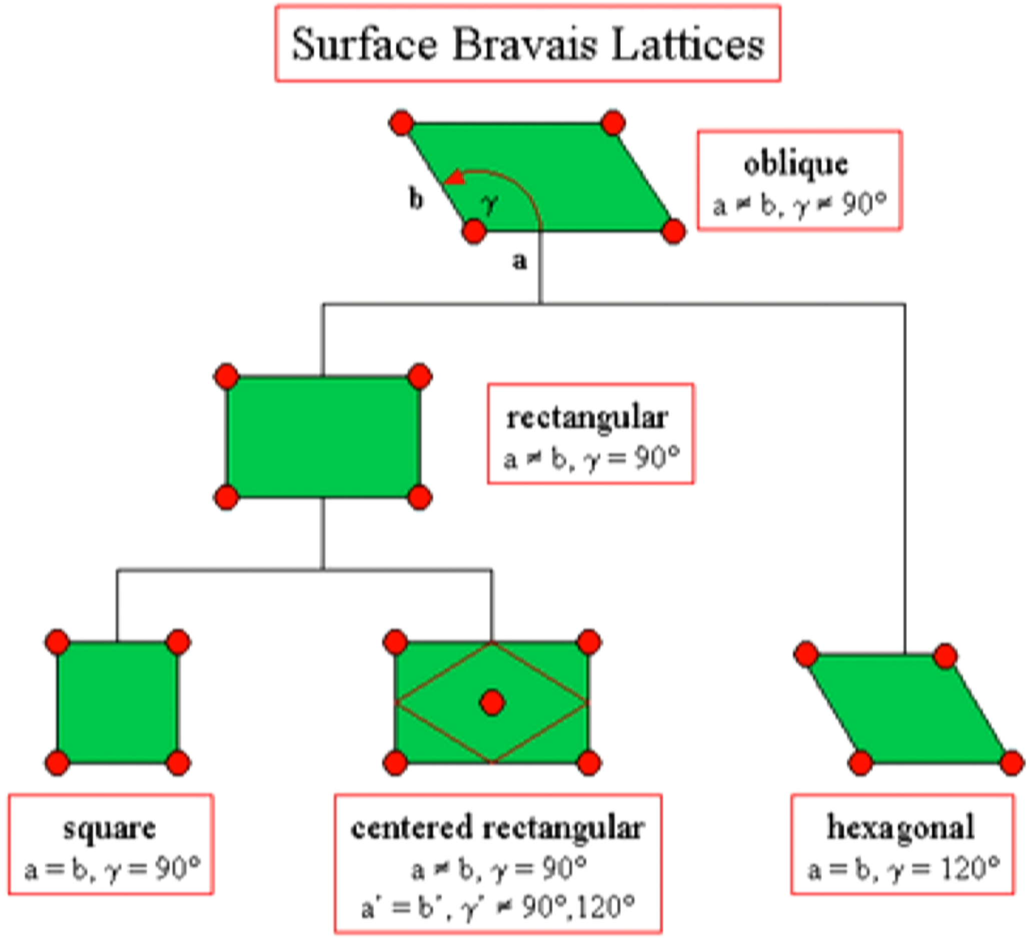
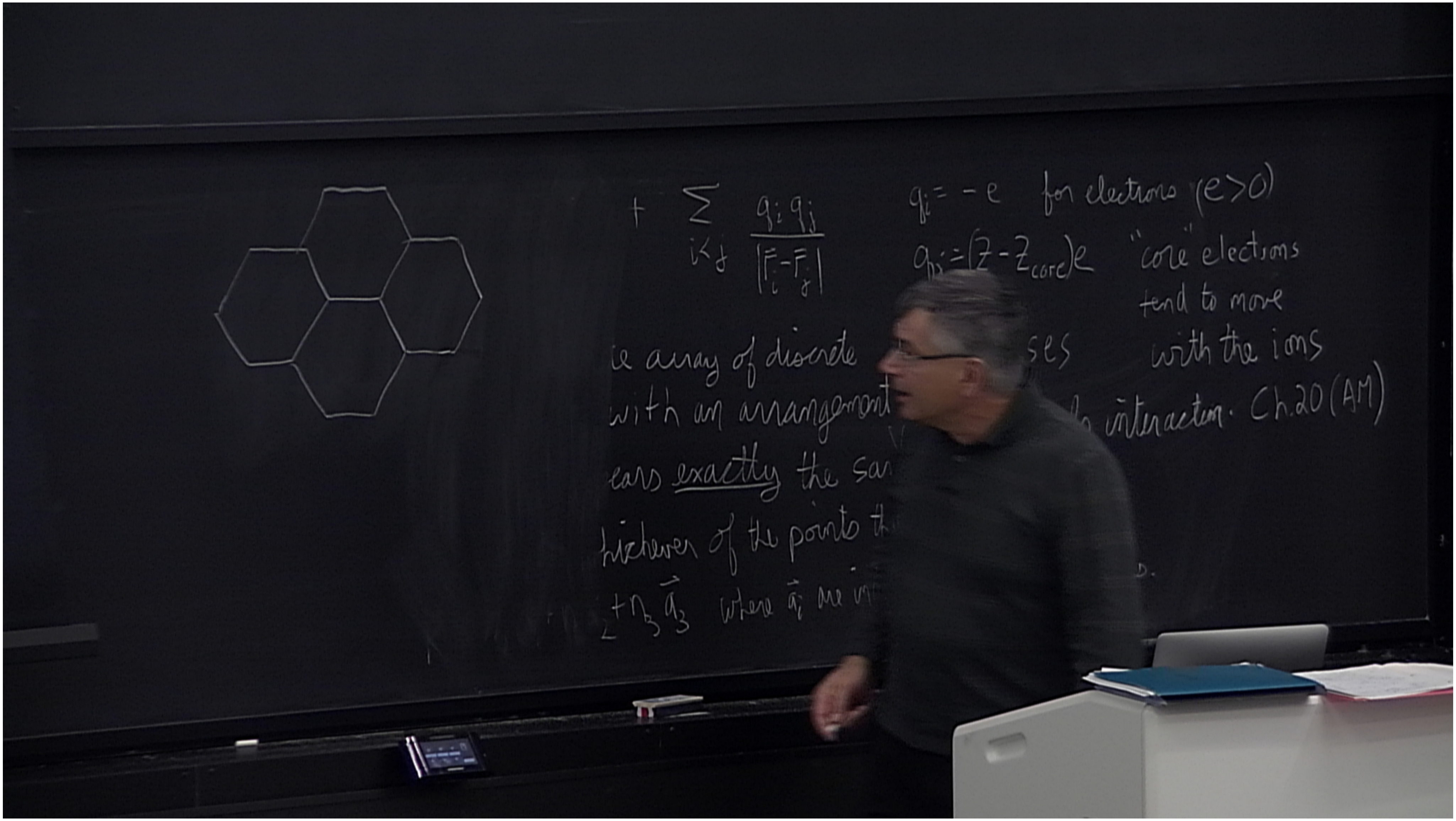
Aschroft and Mermin, p. 72

2D Bravais Lattices



http://pms.iitk.ernet.in/wiki/index.php Unit-1:_Introduction_to_Crystallography


$+ \sum_{i<j} \frac{q_i q_j}{|\vec{r}_i - \vec{r}_j|}$
$q_i = -e$ for electrons $(e>0)$
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"core" electrons
tend to move
with the ions
interaction. Ch.20 (AM)
array of discrete
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exactly the sa
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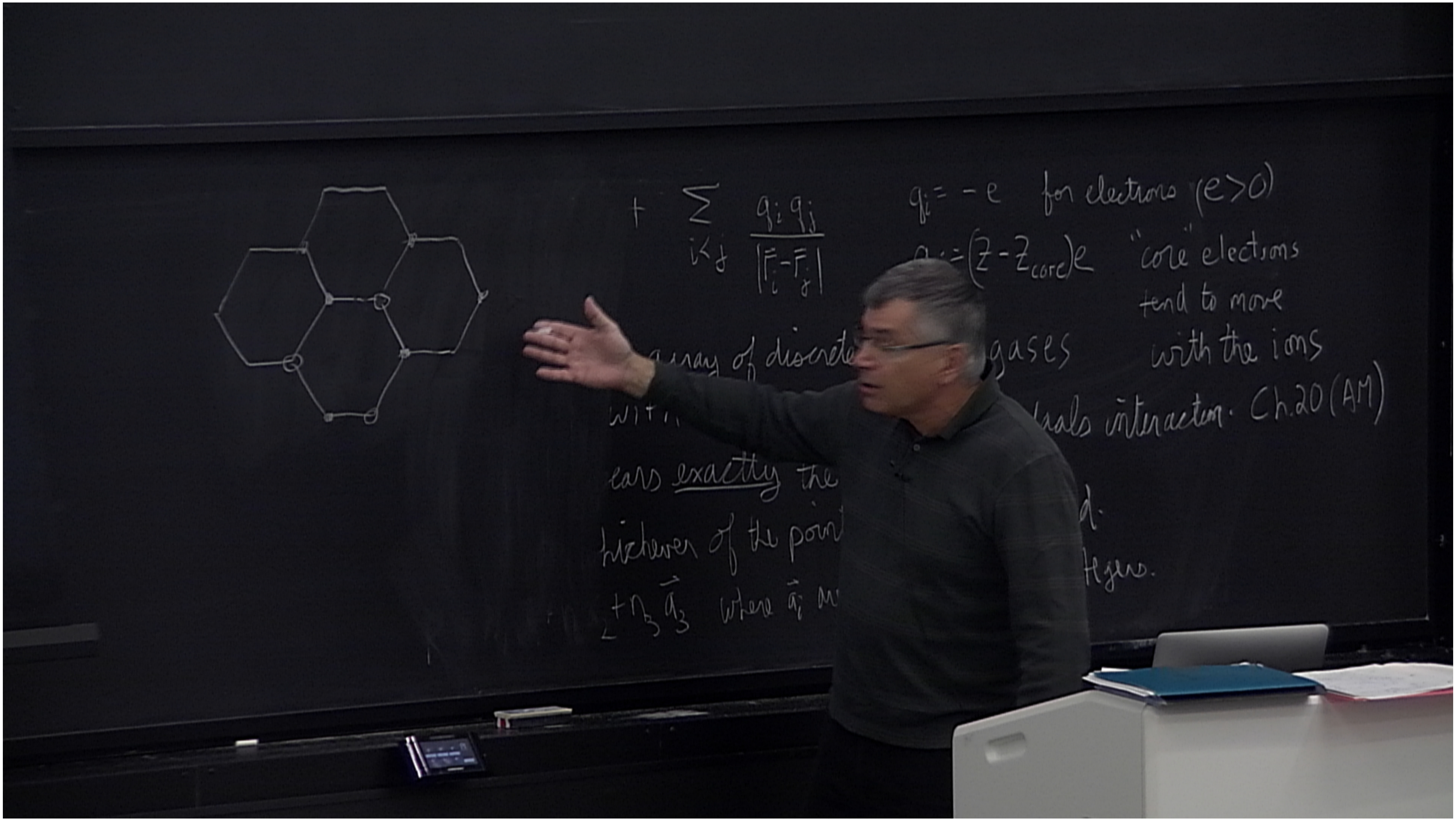
$+n_3\vec{a}_3$ where $\vec{a}_i$ are



$+ \sum_{i<j} \frac{q_i q_j}{|\vec{r}_i - \vec{r}_j|}$
$q_i = -e$ for electrons $(e>0)$
$(Z - Z_{core})e$
"core" electrons
tend to move
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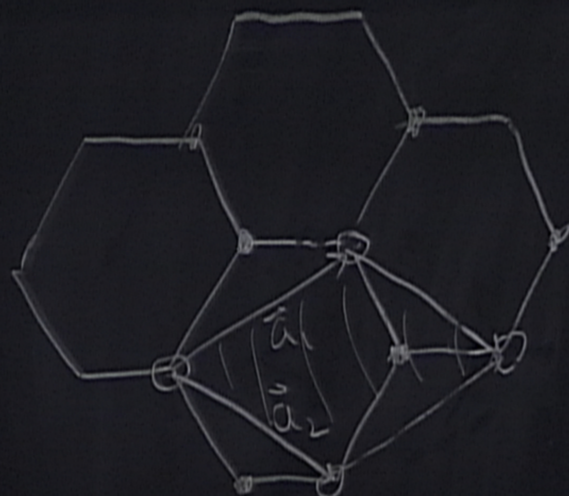


$$+ \sum_{i<j} \frac{q_i q_j}{|\vec{r}_i - \vec{r}_j|} \qquad q_i = -e$$

$q_{\delta} = (Z - \ldots$

...e array of discrete   Noble ga...

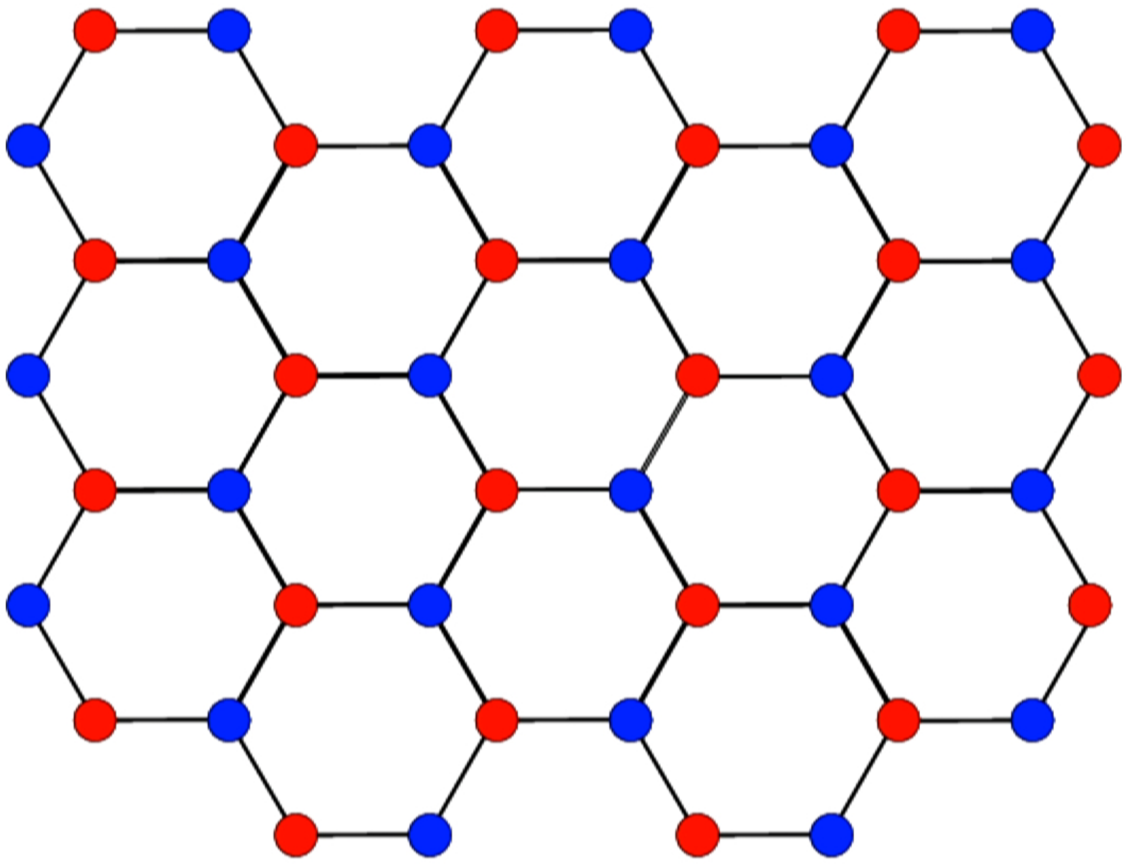
with an arrangement

van der W...

...ears <u>exactly</u> the same,

...hichever of the points the array is ...

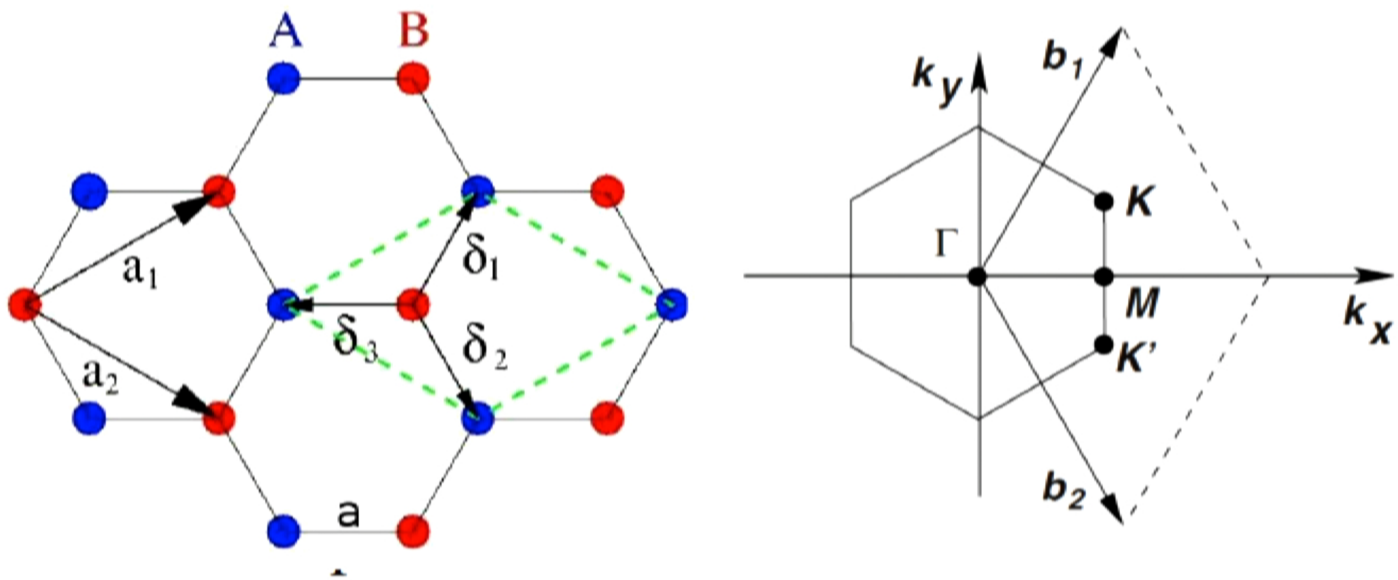
$\ldots_2 + n_3 \vec{a}_3$ where $\vec{a}_i$ are independent, n_i ...



https://inspirehep.net/record/682567/plots

$$\boldsymbol{\delta}_1 = \frac{a}{2}(1, \sqrt{3}) \quad \boldsymbol{\delta}_2 = \frac{a}{2}(1, -\sqrt{3}) \quad \delta_3 = -a(1,0)$$

Castro Neto *et al.*: The electronic properties of graphene
Rev. Mod. Phys., Vol. 81, No. 1, January–March 2009



$$\boldsymbol{a}_1 = \frac{a}{2}(3, \sqrt{3}), \quad \boldsymbol{a}_2 = \frac{a}{2}(3, -\sqrt{3})$$

https://www.researchgate.net/publication/283904445_Weak_Localization_in_Graphene/figures?lo=1

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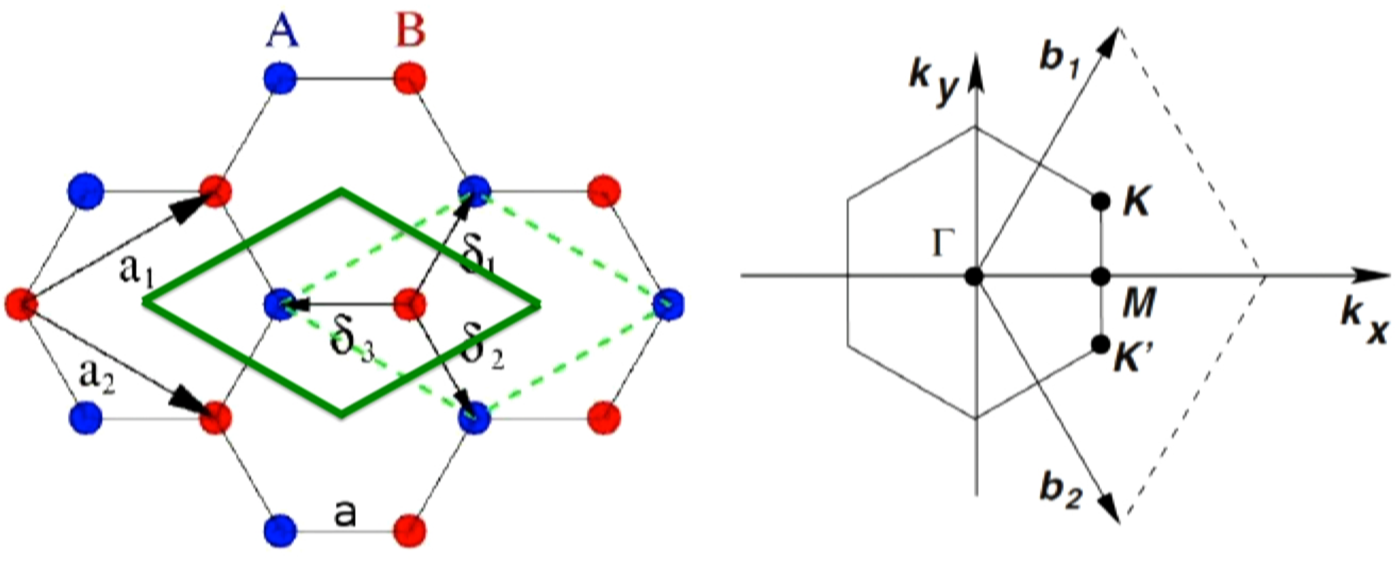

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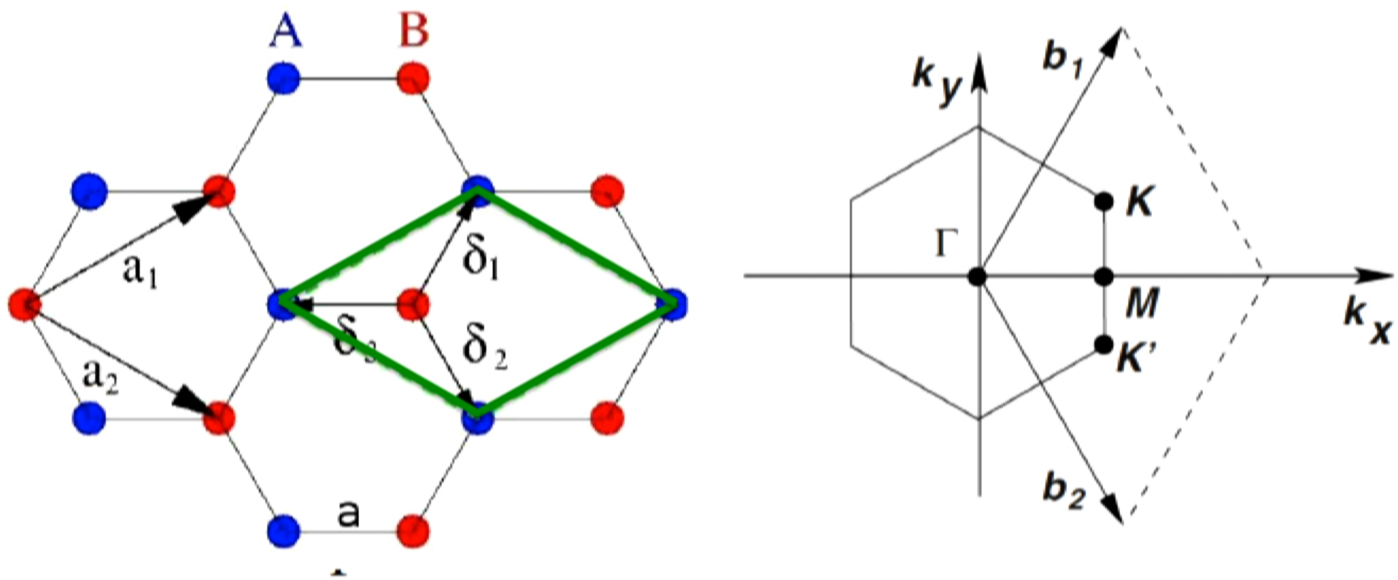

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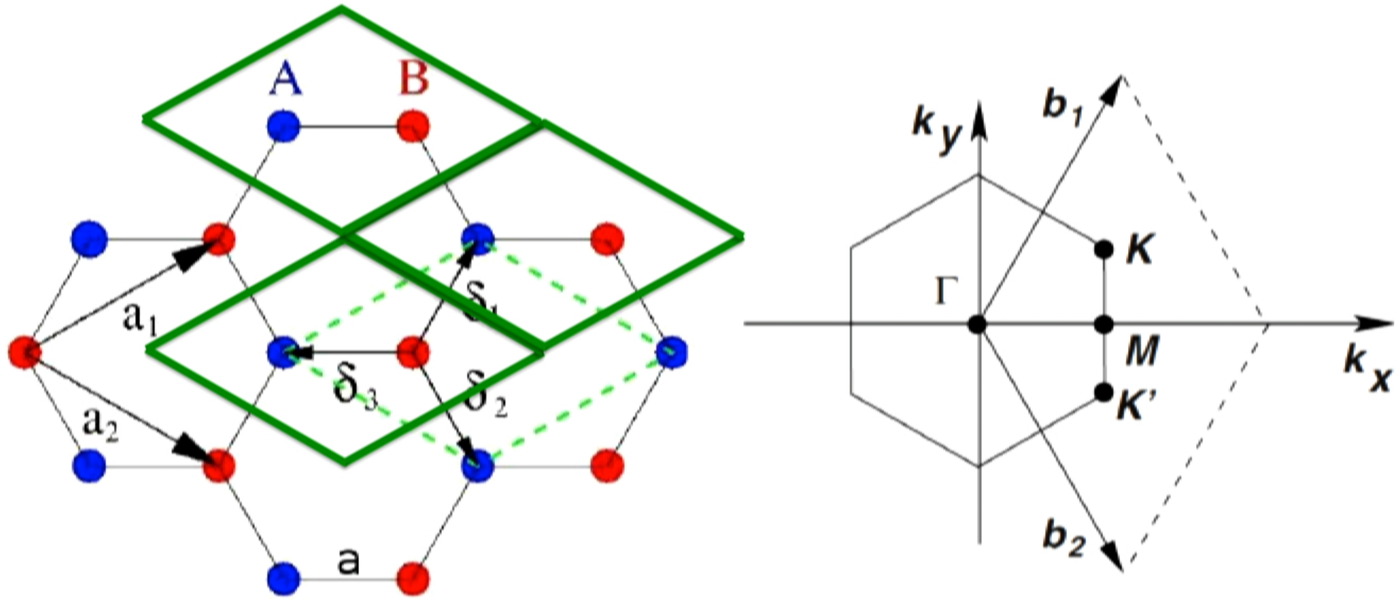

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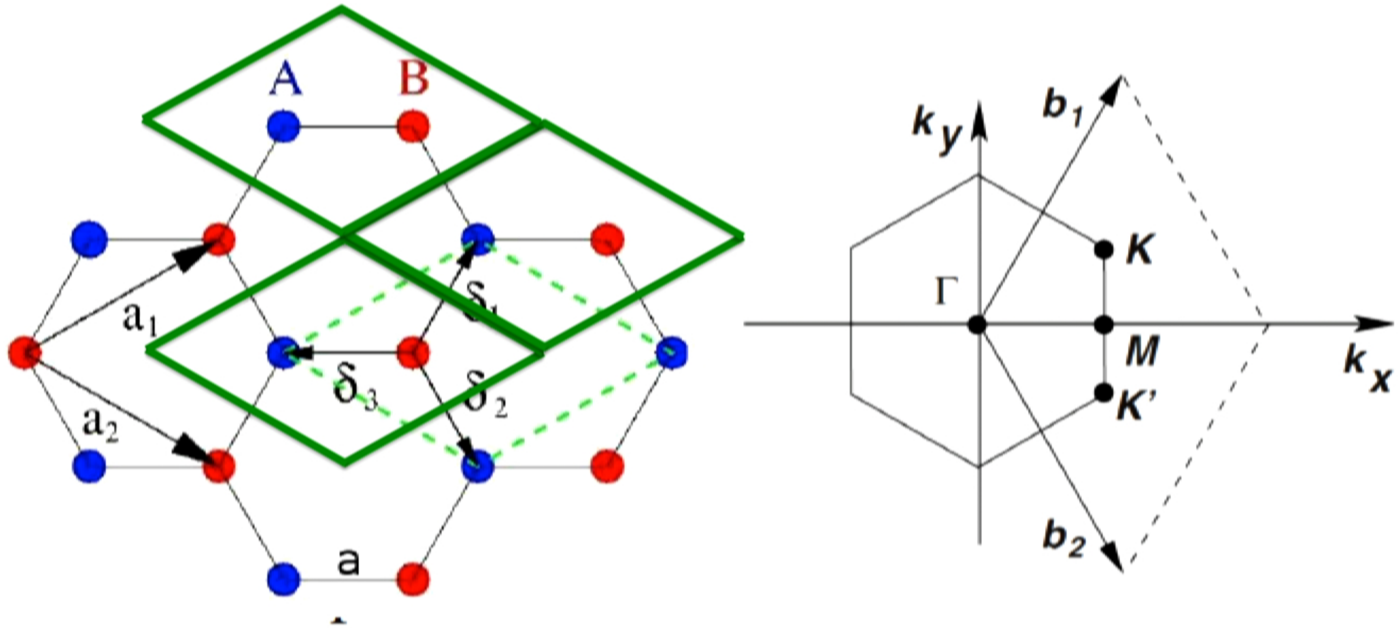

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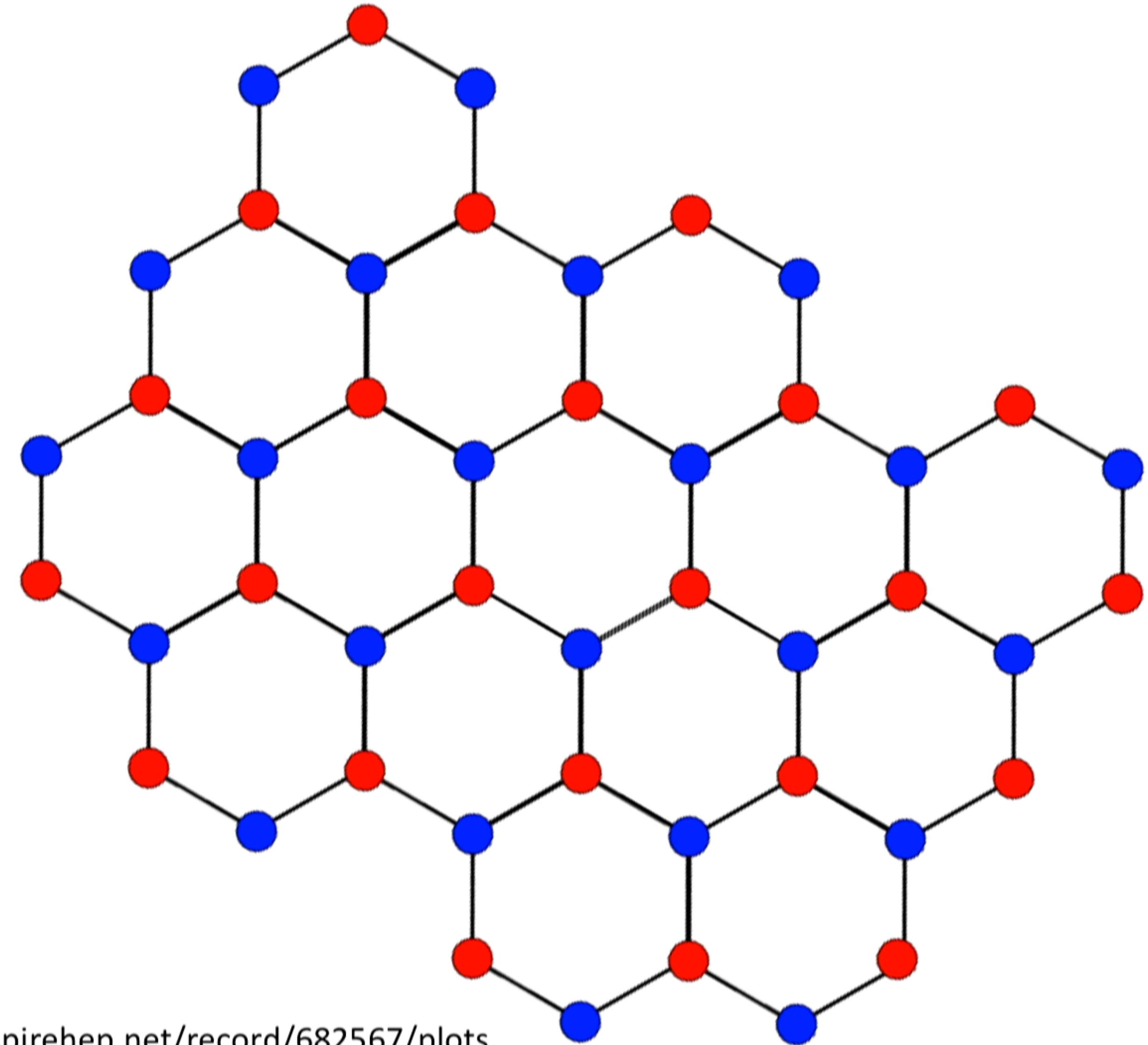

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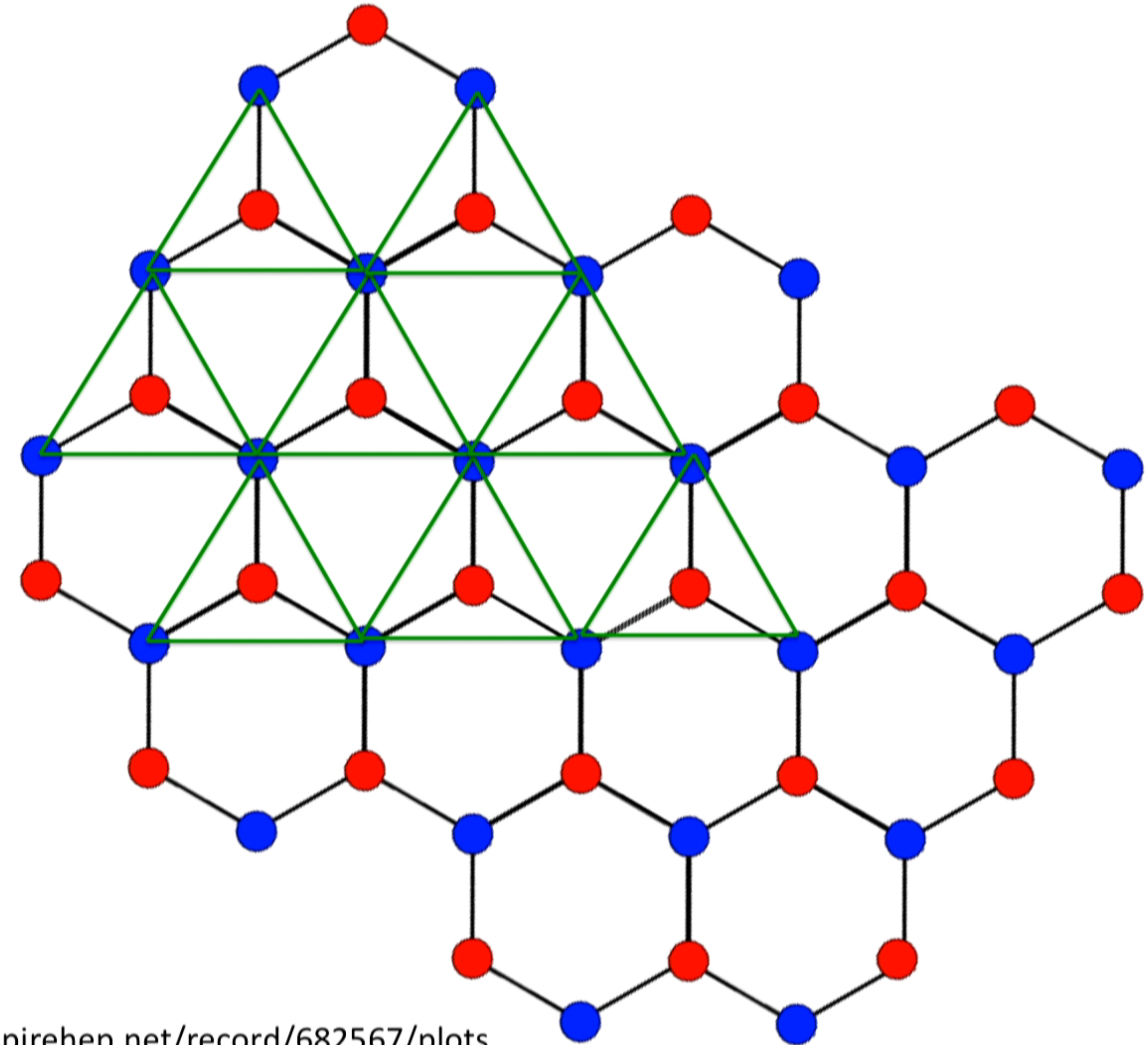

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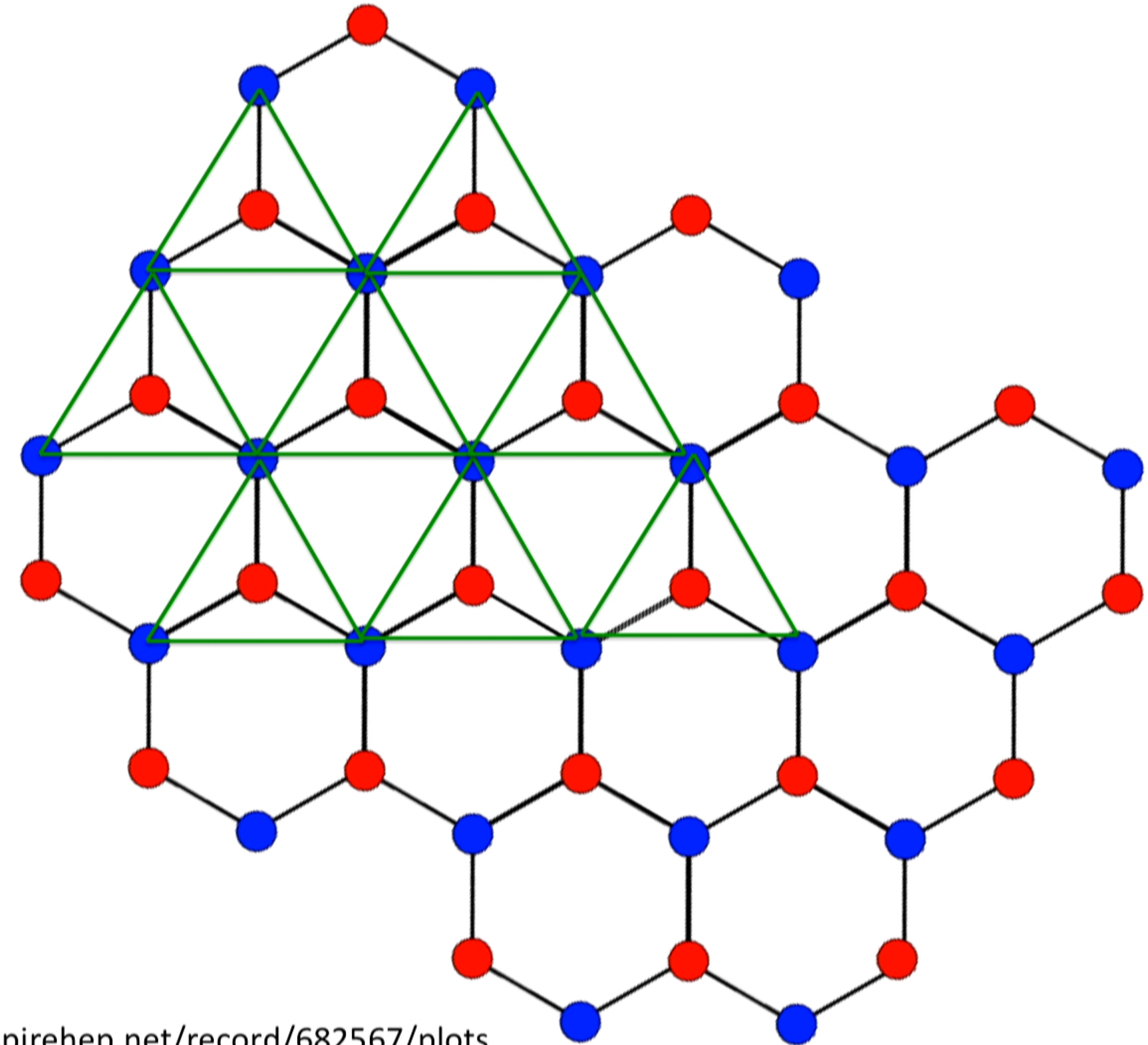

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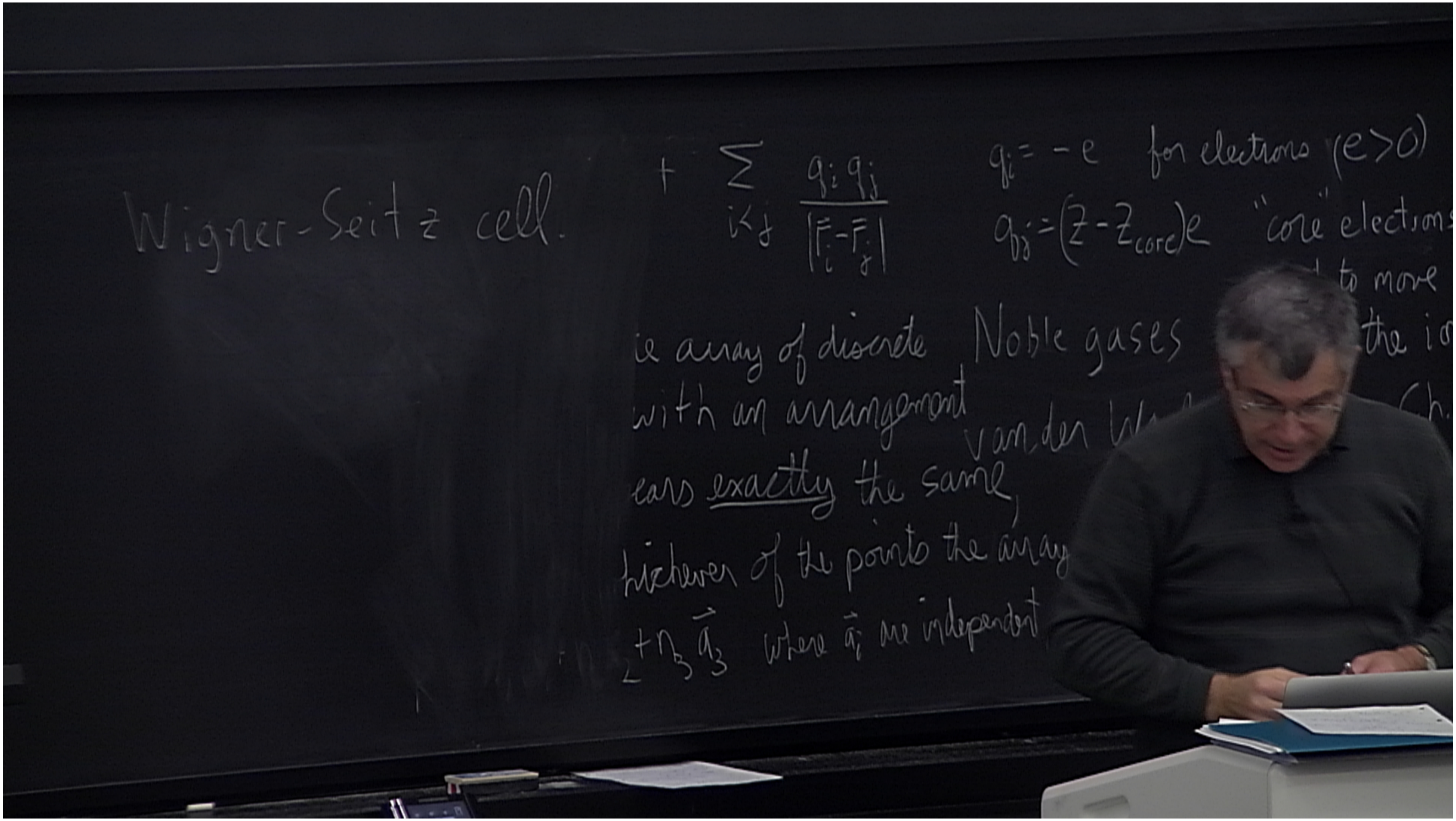
Wigner-Seitz cell.
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van der W
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$_2 + n_3 \vec{a}_3$ where $\vec{a}_i$ are independent

Figure 4.15
The Wigner-Seitz cell for the body-centered cubic Bravais lattice (a "truncated octahedron"). The surrounding cube is a conventional body-centered cubic cell with a lattice point at its center and on each vertex. The hexagonal faces bisect the lines joining the central point to the points on the vertices (drawn as solid lines). The square faces bisect the lines joining the central point to the central points in each of the six neighboring cubic cells (not drawn). The hexagons are regular (see Problem 4d).

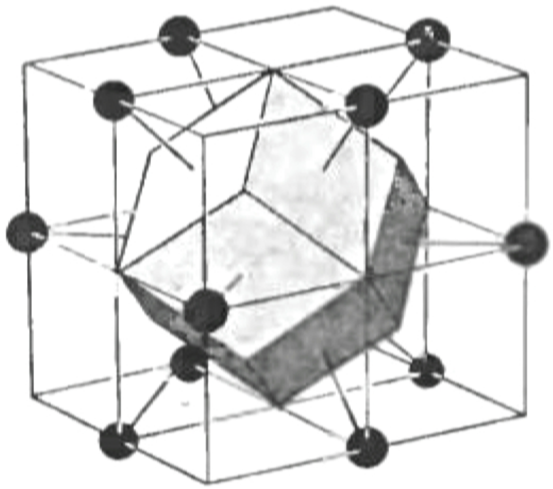
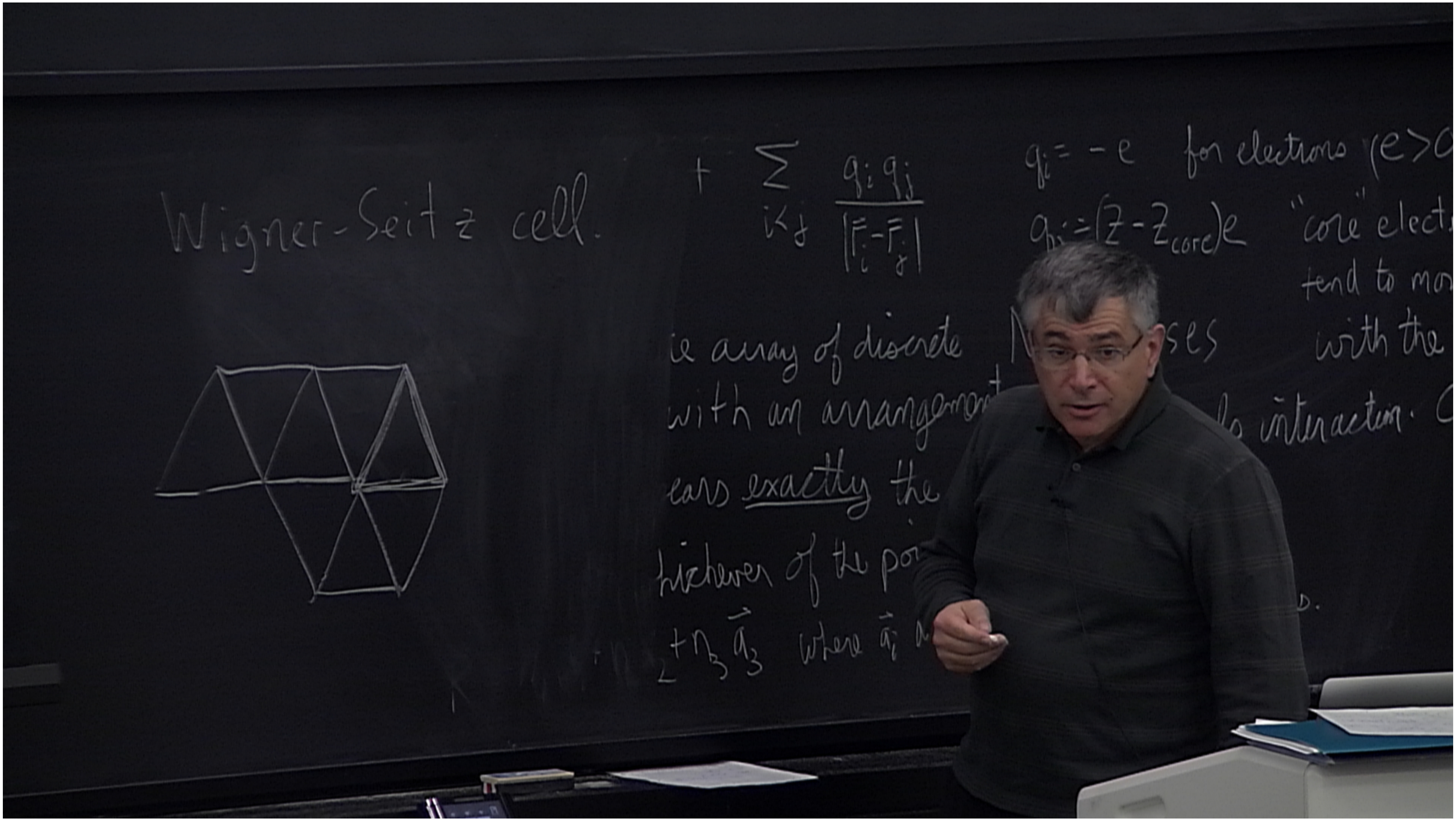


Figure 4.16
Wigner-Seitz cell for the face-centered cubic Bravais lattice (a "rhombic dodecahedron"). The surrounding cube is *not* the conventional cubic cell of Figure 4.12, but one in which lattice points are at the center of the cube and at the center of the 12 edges. Each of the 12 (congruent) faces is perpendicular to a line joining the central point to a point on the center of an edge.

Aschroft and Mermin, p. 74


Wigner-Seitz cell.
$+ \sum_{i<j} \frac{q_i q_j}{|\vec{r}_i - \vec{r}_j|}$
$q_i = -e$ for electrons
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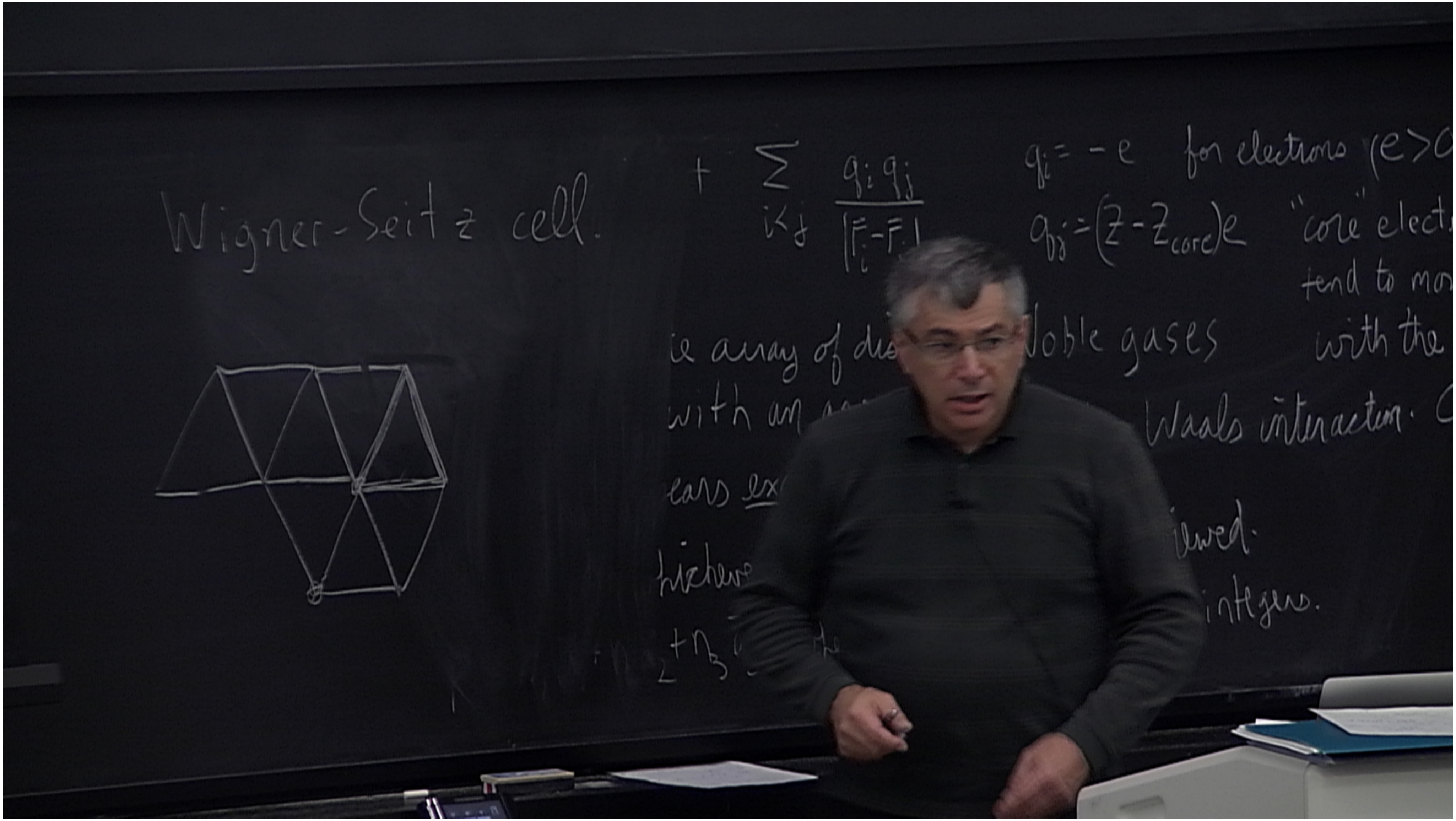
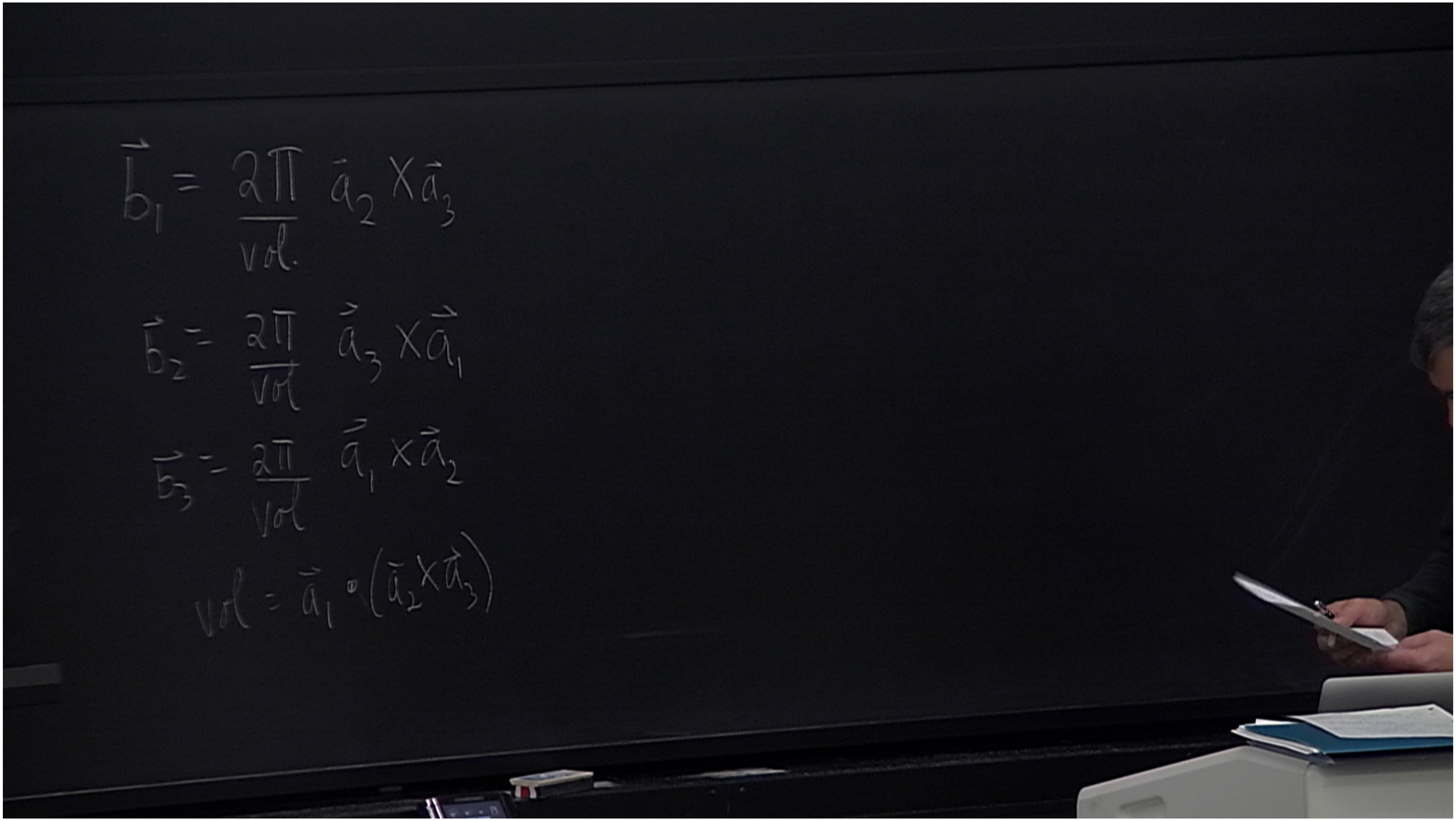

Wigner-Seitz cell.
q_i = -e for electrons
q_γ = (Z - Z_core) e
Waals interaction.
integers.


$\vec{b}_1 = \frac{2\pi}{vol.} \vec{a}_2 \times \vec{a}_3$
$\vec{b}_2 = \frac{2\pi}{vol} \vec{a}_3 \times \vec{a}_1$
$\vec{b}_3 = \frac{2\pi}{vol} \vec{a}_1 \times \vec{a}_2$
$vol = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$

$$\vec{b}_1 = \frac{2\pi}{vol.}\, \vec{a}_2 \times \vec{a}_3$$

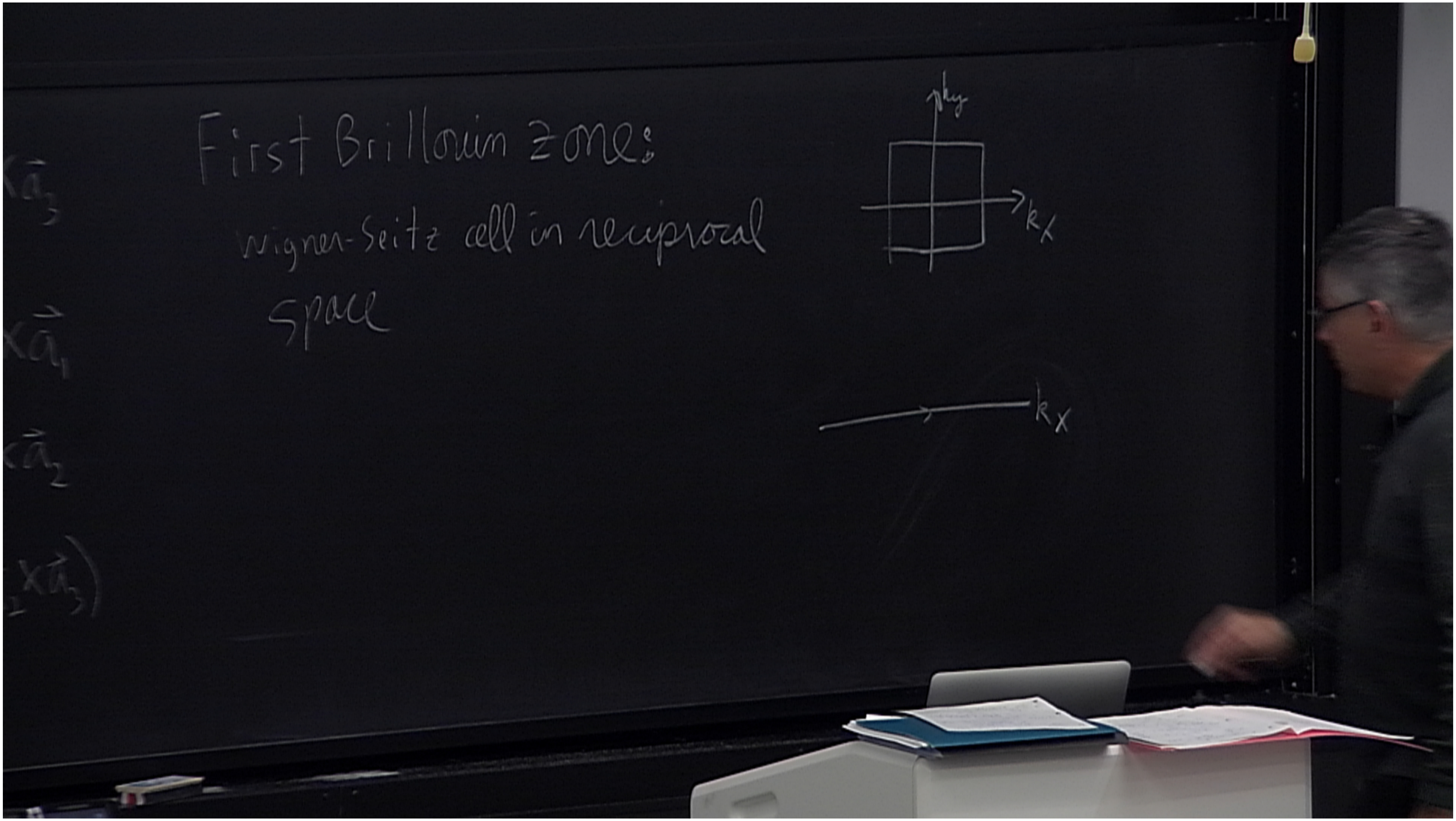
$$\vec{b}_2 = \frac{2\pi}{vol}\, \vec{a}_3 \times \vec{a}_1$$

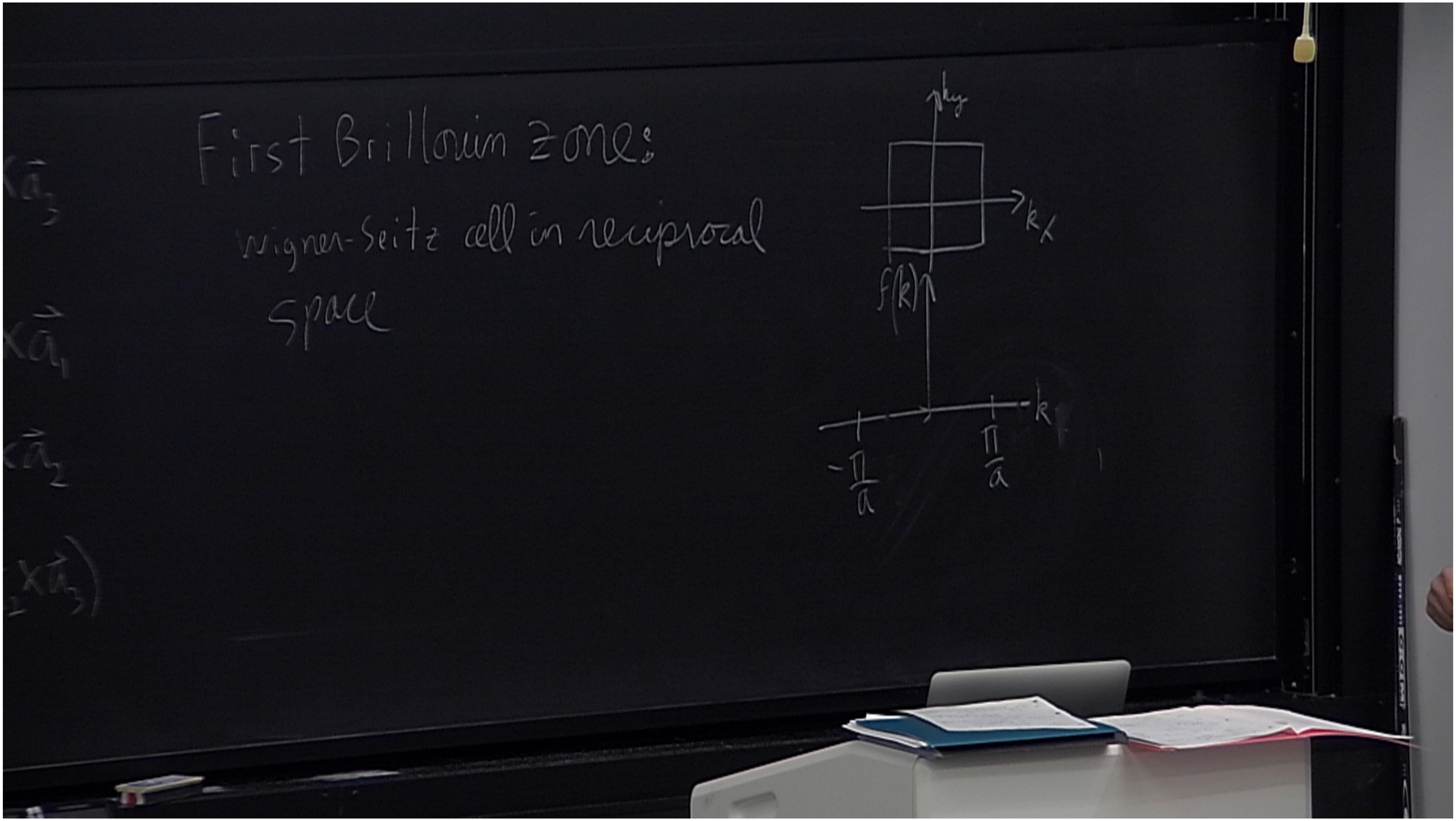
$$\vec{b}_3 = \frac{2\pi}{vol}\, \vec{a}_1 \times \vec{a}_2$$

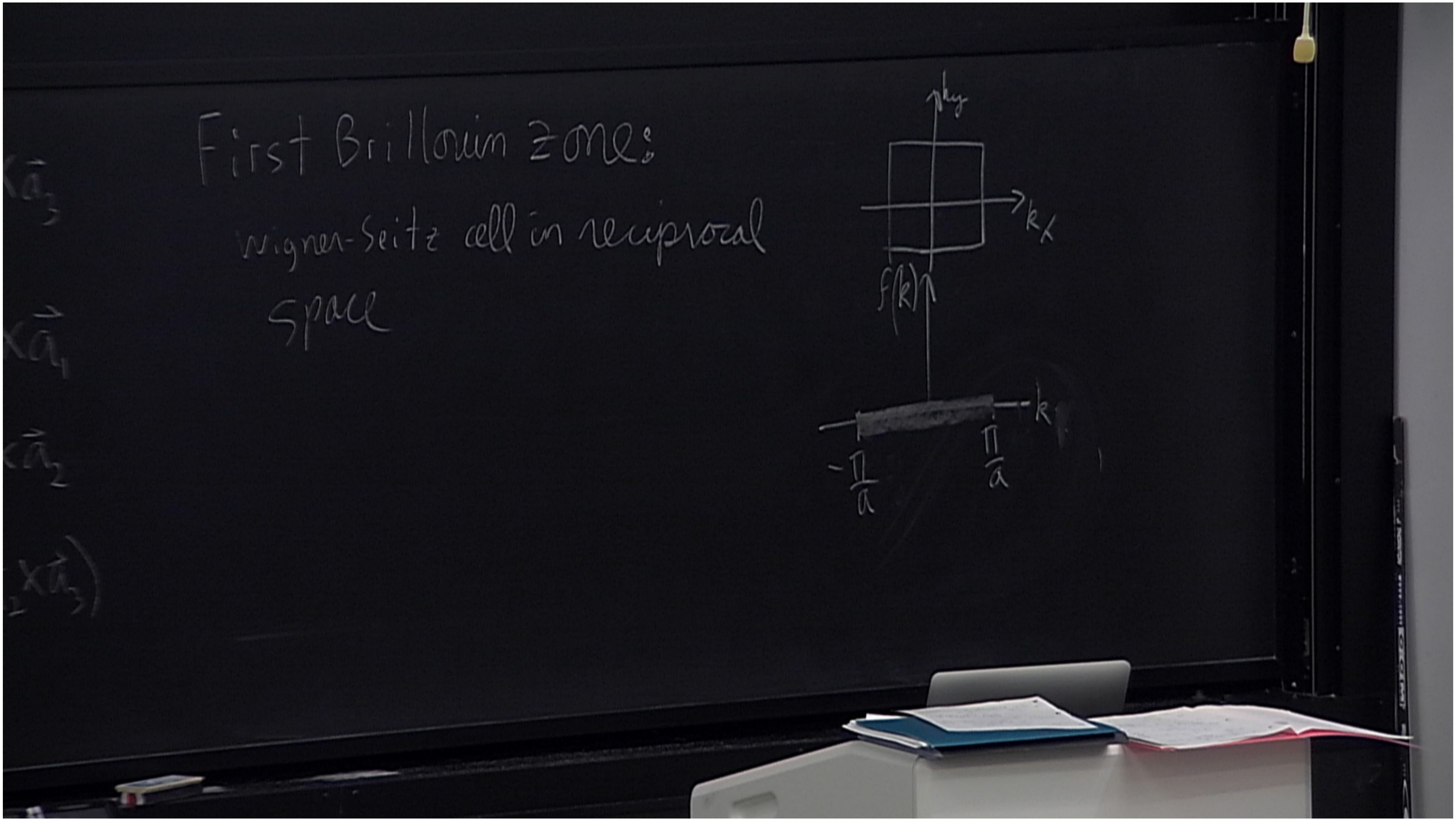
$$vol = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$$

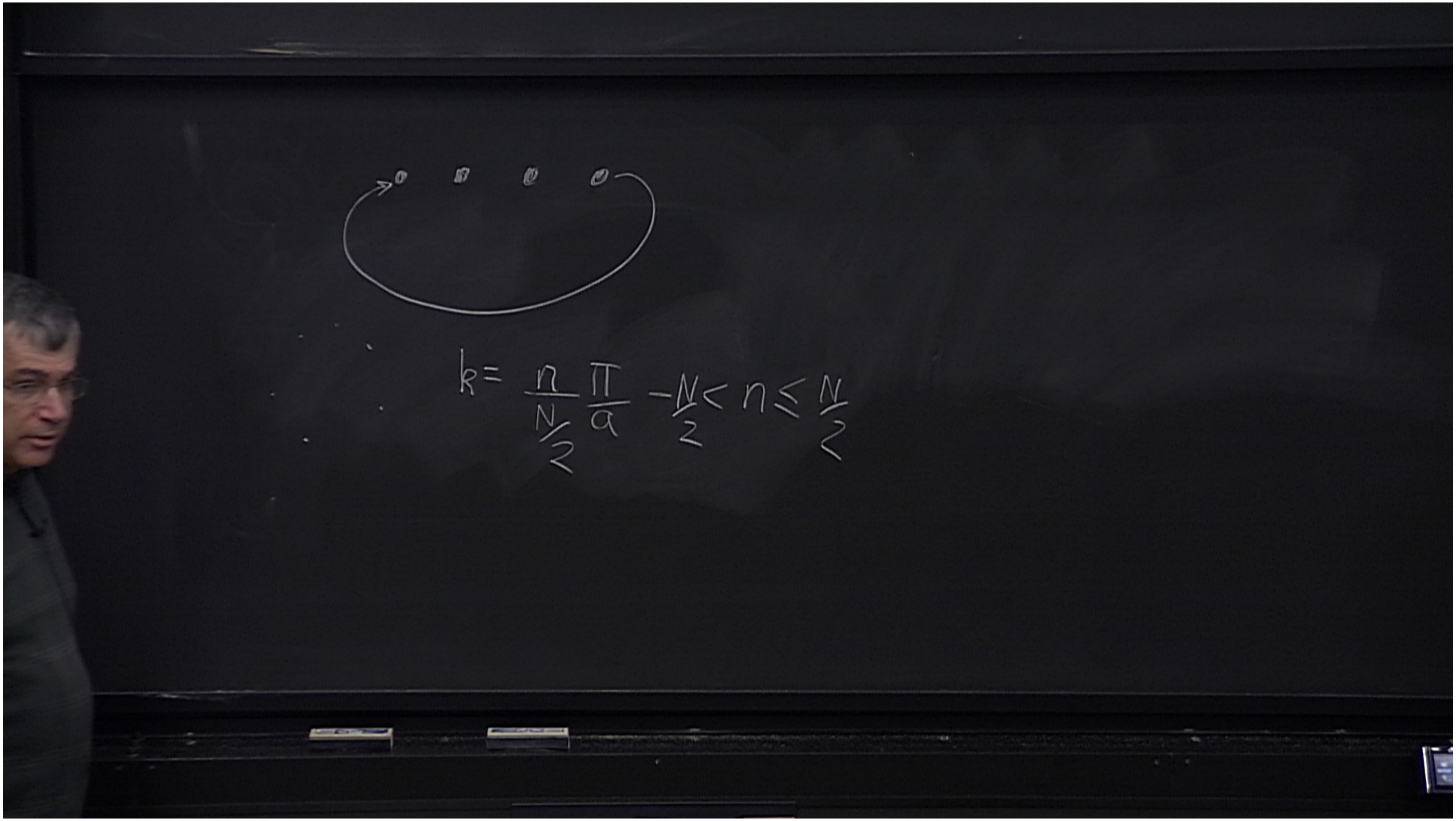
First Brillouin zone:

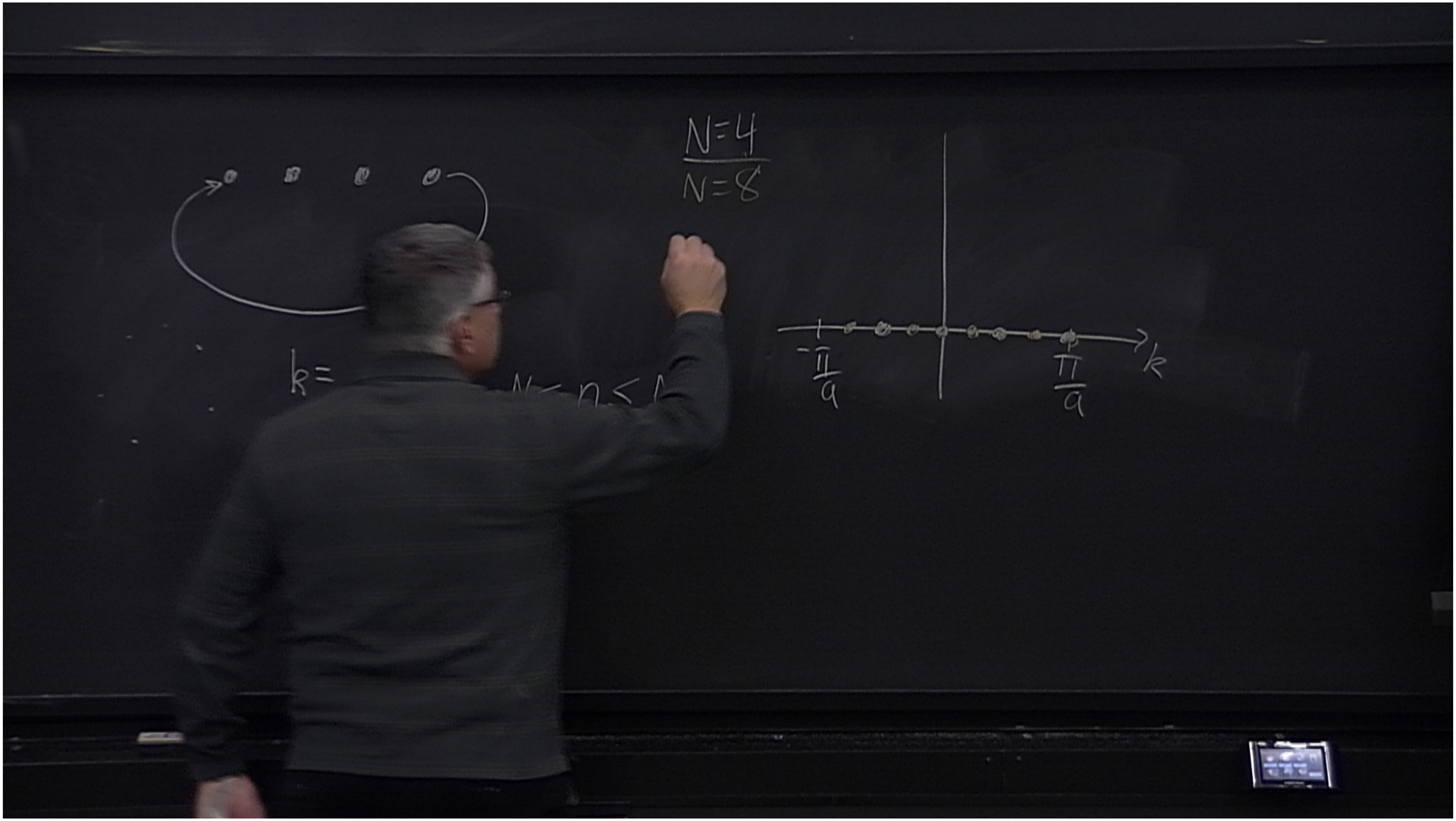
Wigner-Seitz cell in reciprocal space

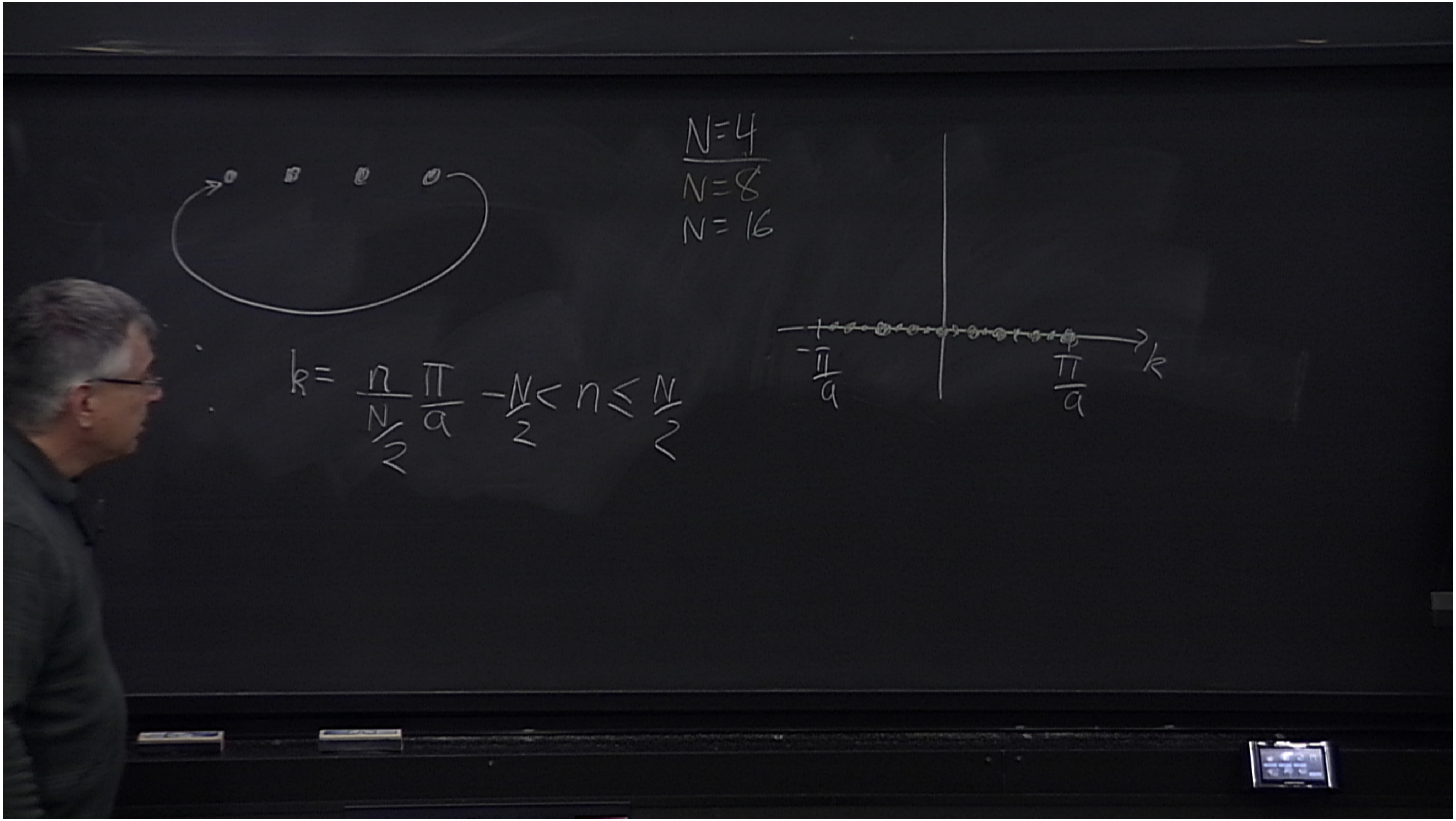

First Brillouin zone:
Wigner-Seitz cell in reciprocal space
k_y
k_x
k_x

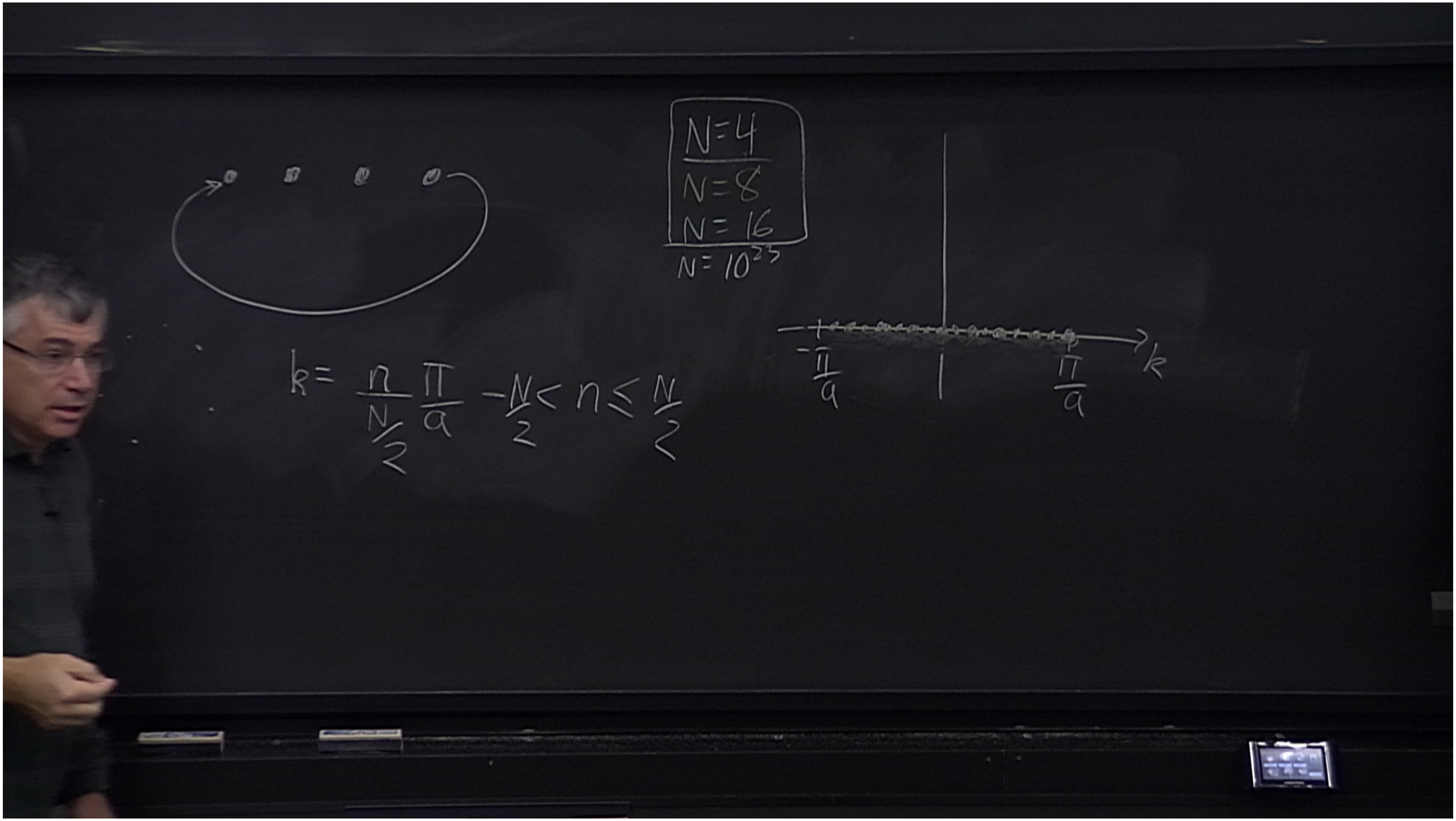

First Brillouin zone:
Wigner-Seitz cell in reciprocal space
ky
kx
f(k)
k
-π/a
π/a

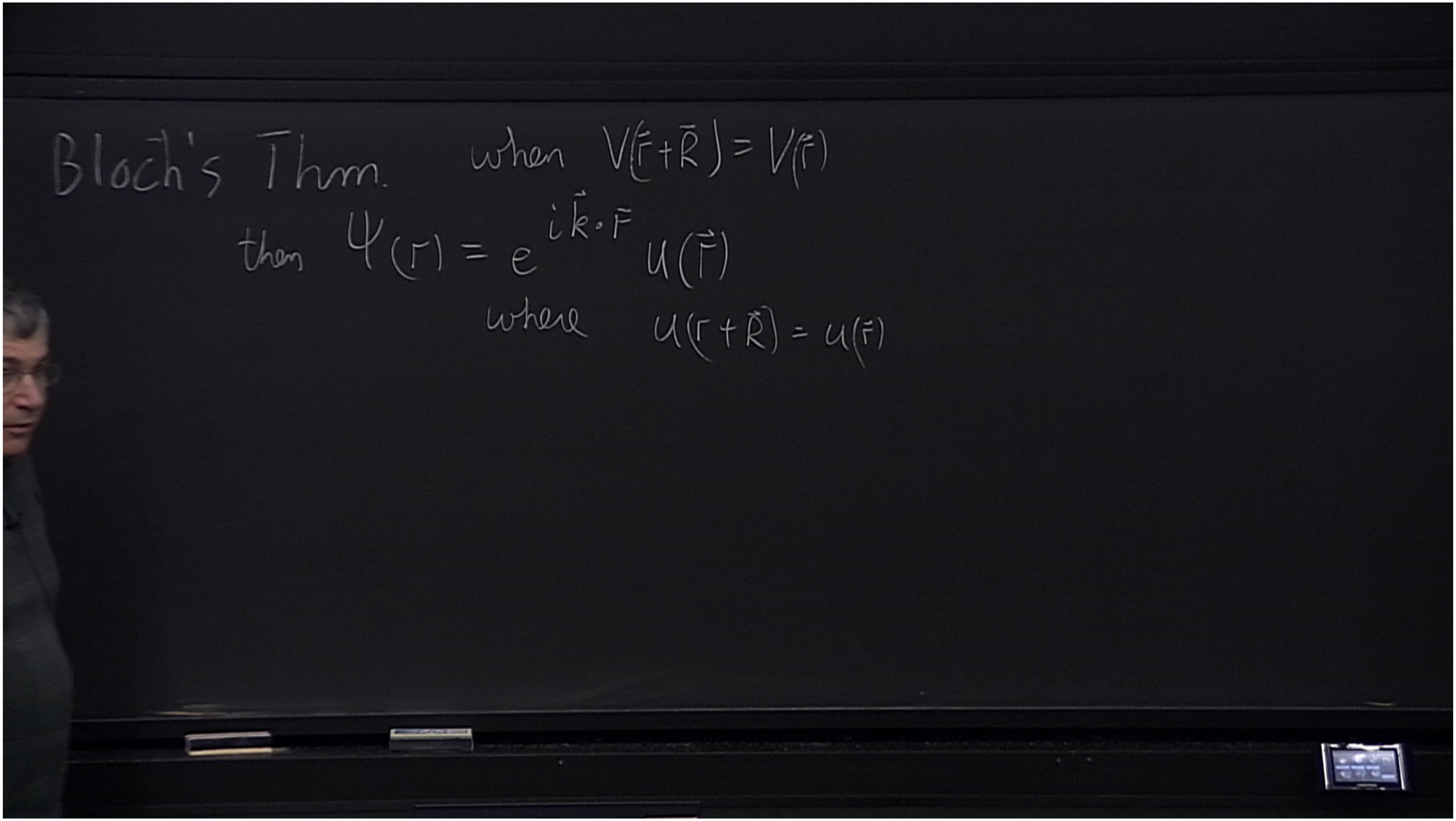

First Brillouin zone:
Wigner-Seitz cell in reciprocal space
k_y
k_x
$f(k)$
k
$-\frac{\pi}{a}$
$\frac{\pi}{a}$

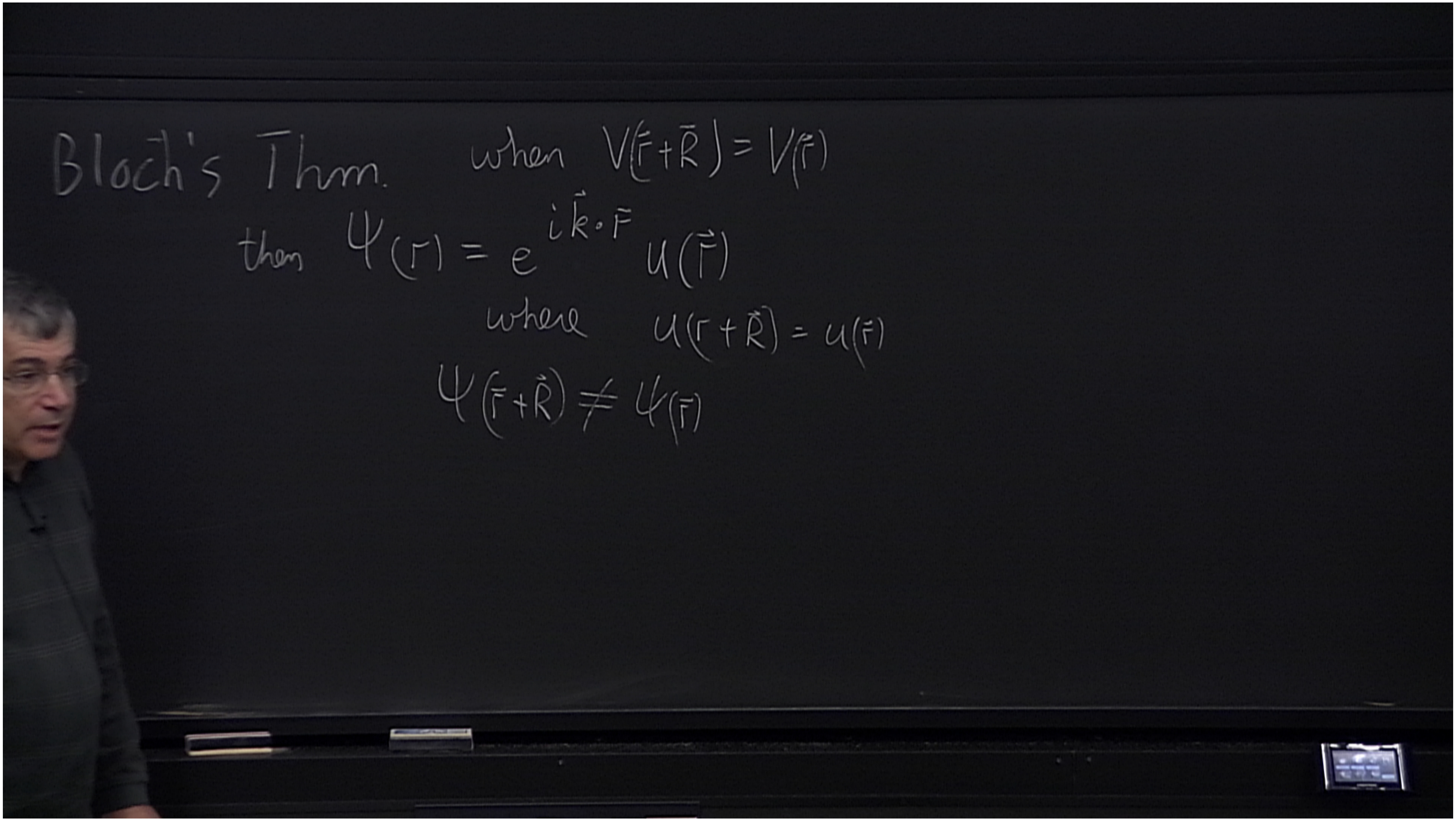

$k = \frac{n}{N/2}\frac{\pi}{a}$ $-\frac{N}{2} < n \leq \frac{N}{2}$


N=4
N=8
k=
k


N=4
N=8
N=16
k = n/(N/2) π/a
-N/2 < n ≤ N/2
-π/a
π/a
k


N=4
N=8
N=16
N=10^23
k= n/(N/2) π/a
-N/2 < n ≤ N/2
-π/a
π/a
k


Bloch's Thm. when $V(\vec{r}+\vec{R}) = V(\vec{r})$
then $\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u(\vec{r})$
where $u(\vec{r}+\vec{R}) = u(\vec{r})$


Bloch's Thm. when $V(\vec{r}+\vec{R}) = V(\vec{r})$
then $\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u(\vec{r})$
where $u(\vec{r}+\vec{R}) = u(\vec{r})$
$\psi(\vec{r}+\vec{R}) \neq \psi(\vec{r})$

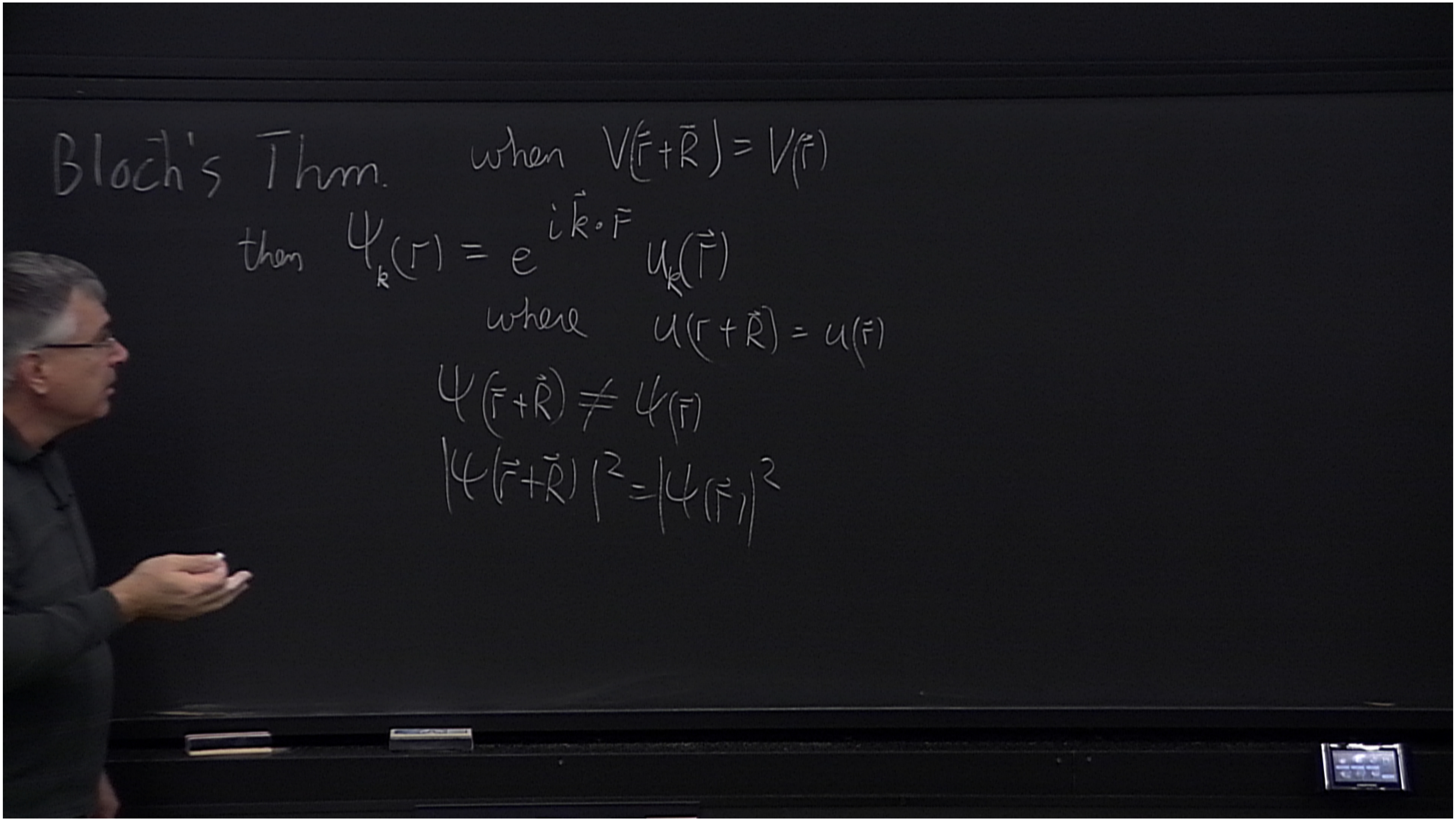
Bloch's Thm. when $V(\vec{r}+\vec{R}) = V(\vec{r})$

then $\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u(\vec{r})$

where $u(\vec{r}+\vec{R}) = u(\vec{r})$

$$\psi(\vec{r}+\vec{R}) \neq \psi(\vec{r})$$

$$|\psi(\vec{r}+\vec{R})|^2 = |\psi(\vec{r})|^2$$


Bloch's Thm. when $V(\vec{r}+\vec{R}) = V(\vec{r})$
then $\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_k(\vec{r})$
where $u(\vec{r}+\vec{R}) = u(\vec{r})$
$\psi(\vec{r}+\vec{R}) \neq \psi(\vec{r})$
$|\psi(\vec{r}+\vec{R})|^2 = |\psi(\vec{r})|^2$

Bloch's Thm. when $V(\vec{r}+\vec{R}) = V(\vec{r})$

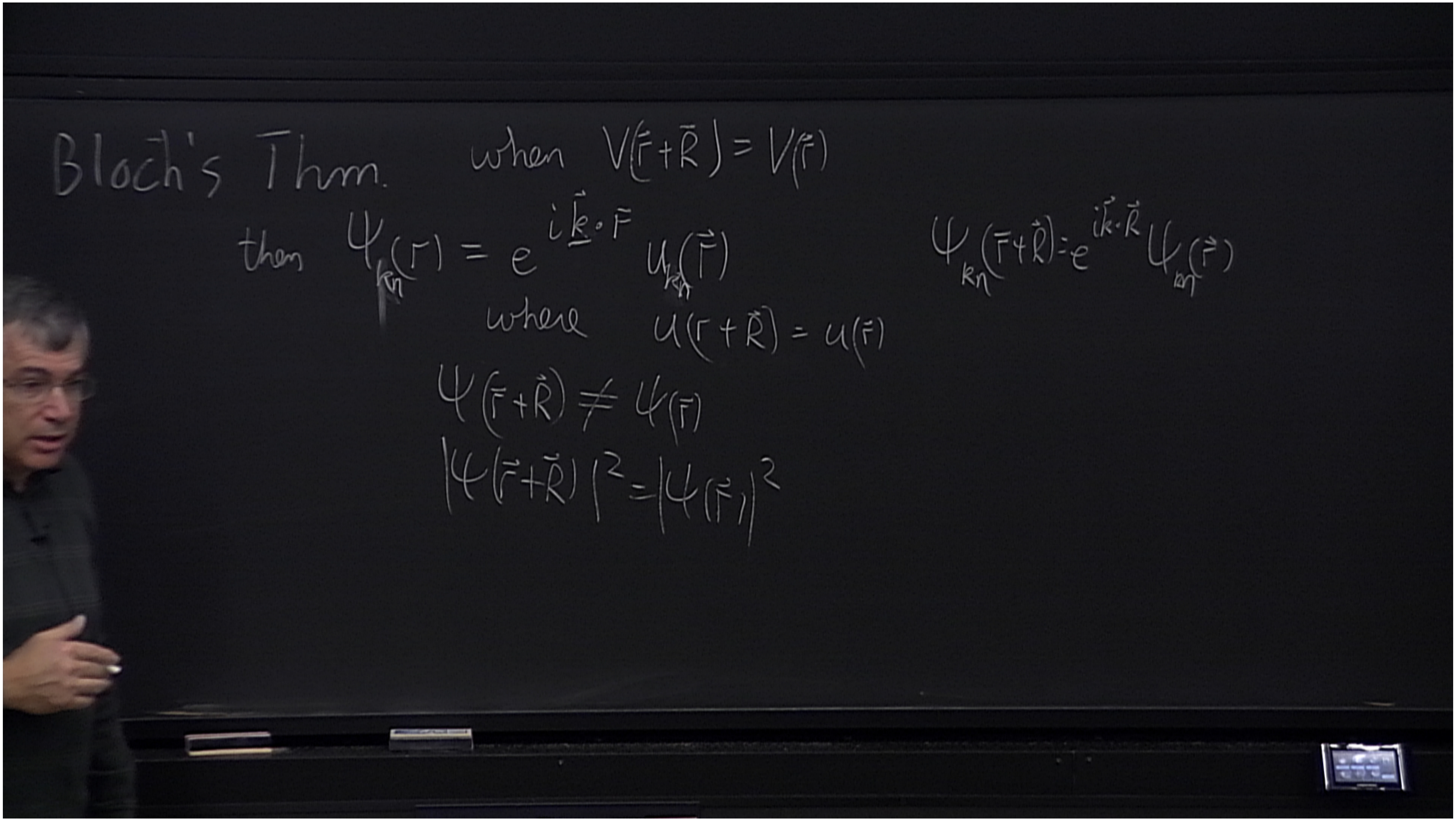
then $\psi_k(\vec{r}) = e^{i\underline{k}\cdot\vec{r}}\, u_k(\vec{r})$

$\psi_k(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}}\,\psi_k(\vec{r})$

where $u(\vec{r}+\vec{R}) = u(\vec{r})$

$$\psi(\vec{r}+\vec{R}) \neq \psi(\vec{r})$$

$$|\psi(\vec{r}+\vec{R})|^2 = |\psi(\vec{r})|^2$$


Bloch's Thm. when $V(\vec{r}+\vec{R}) = V(\vec{r})$
then $\psi_{kn}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{kn}(\vec{r})$
where $u(\vec{r}+\vec{R}) = u(\vec{r})$
$\psi(\vec{r}+\vec{R}) \neq \psi(\vec{r})$
$|\psi(\vec{r}+\vec{R})|^2 = |\psi(\vec{r})|^2$
$\psi_{kn}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}} \psi_{kn}(\vec{r})$

Bloch's Thm. when $V(\vec{r}+\vec{R}) = V(\vec{r})$

then $\psi_{kn}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{kn}(\vec{r})$

where $u(\vec{r}+\vec{R}) = u(\vec{r})$

$$\psi(\vec{r}+\vec{R}) \neq \psi(\vec{r})$$

$$|\psi(\vec{r}+\vec{R})|^2 = |\psi(\vec{r})|^2$$

$$\psi_{kn}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}}\,\psi_{kn}(\vec{r})$$

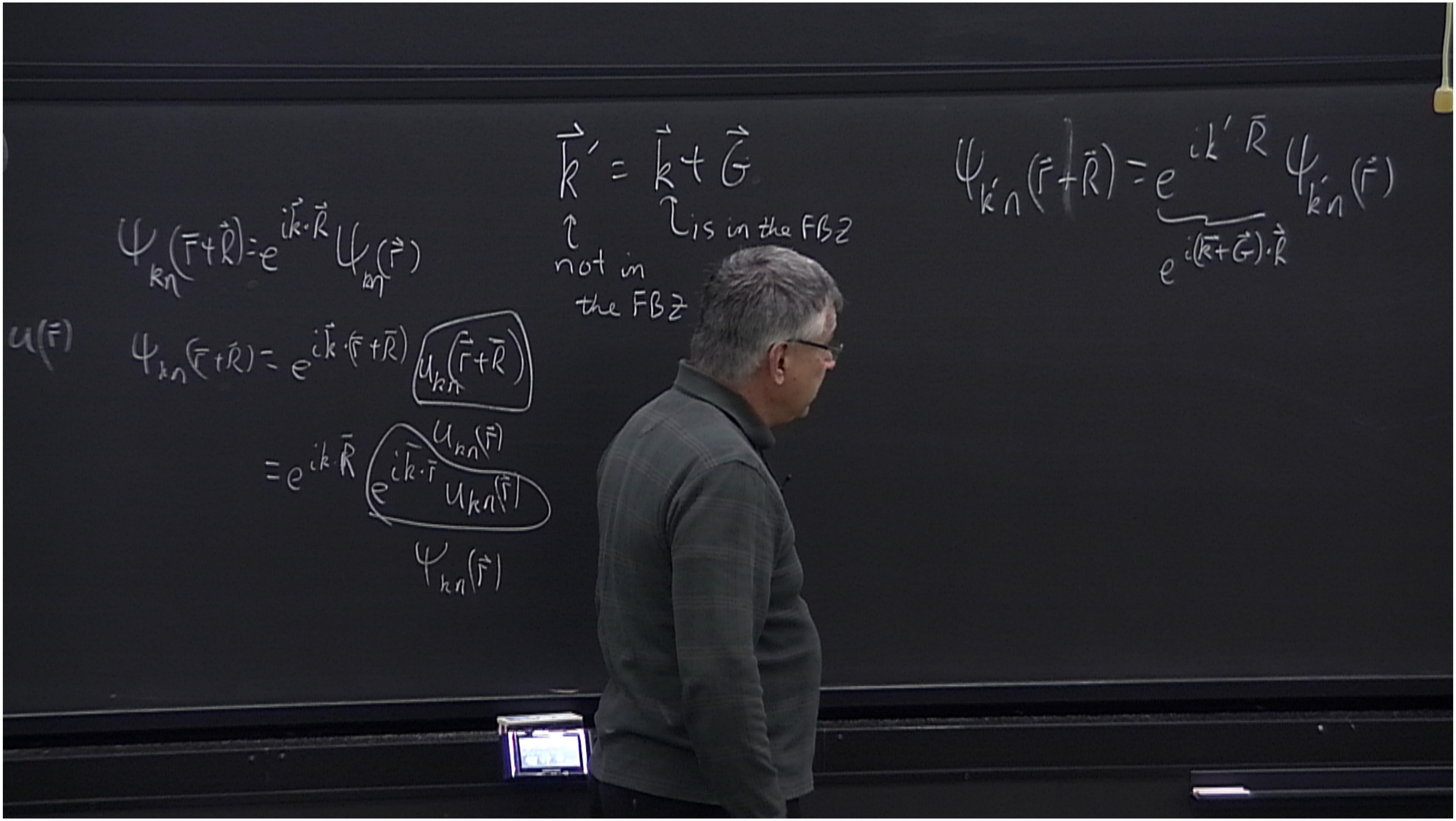
$$\psi_{kn}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot(\vec{r}+\vec{R})}\,\underbrace{u_{kn}(\vec{r}+\vec{R})}_{u_{kn}(\vec{r})}$$

$$= e^{i\vec{k}\cdot\vec{R}}\,\underbrace{e^{i\vec{k}\cdot\vec{r}}\,u_{kn}(\vec{r})}_{\psi_{kn}(\vec{r})}$$

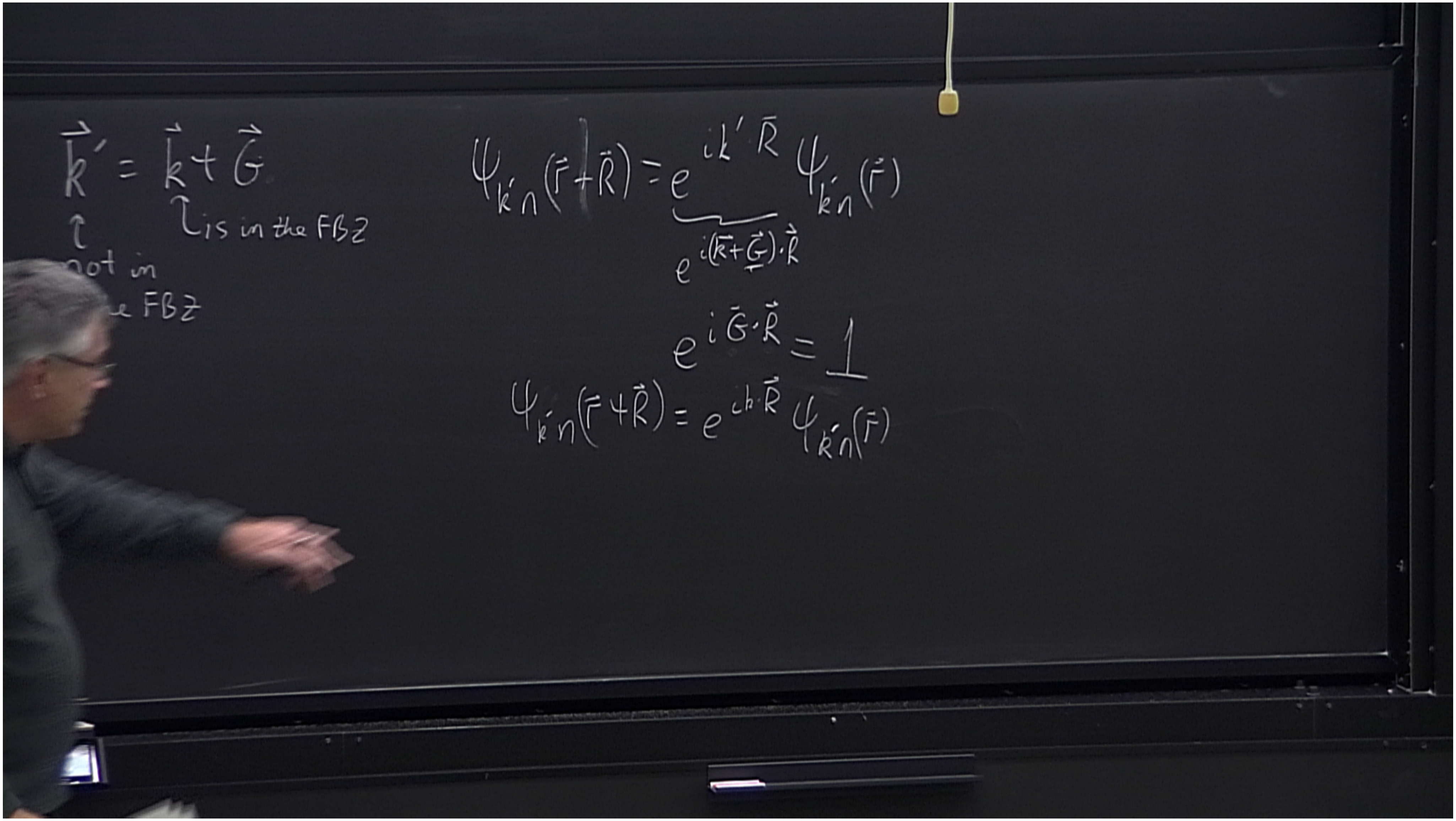
$$\vec{k}' = \vec{k} + \vec{G}$$

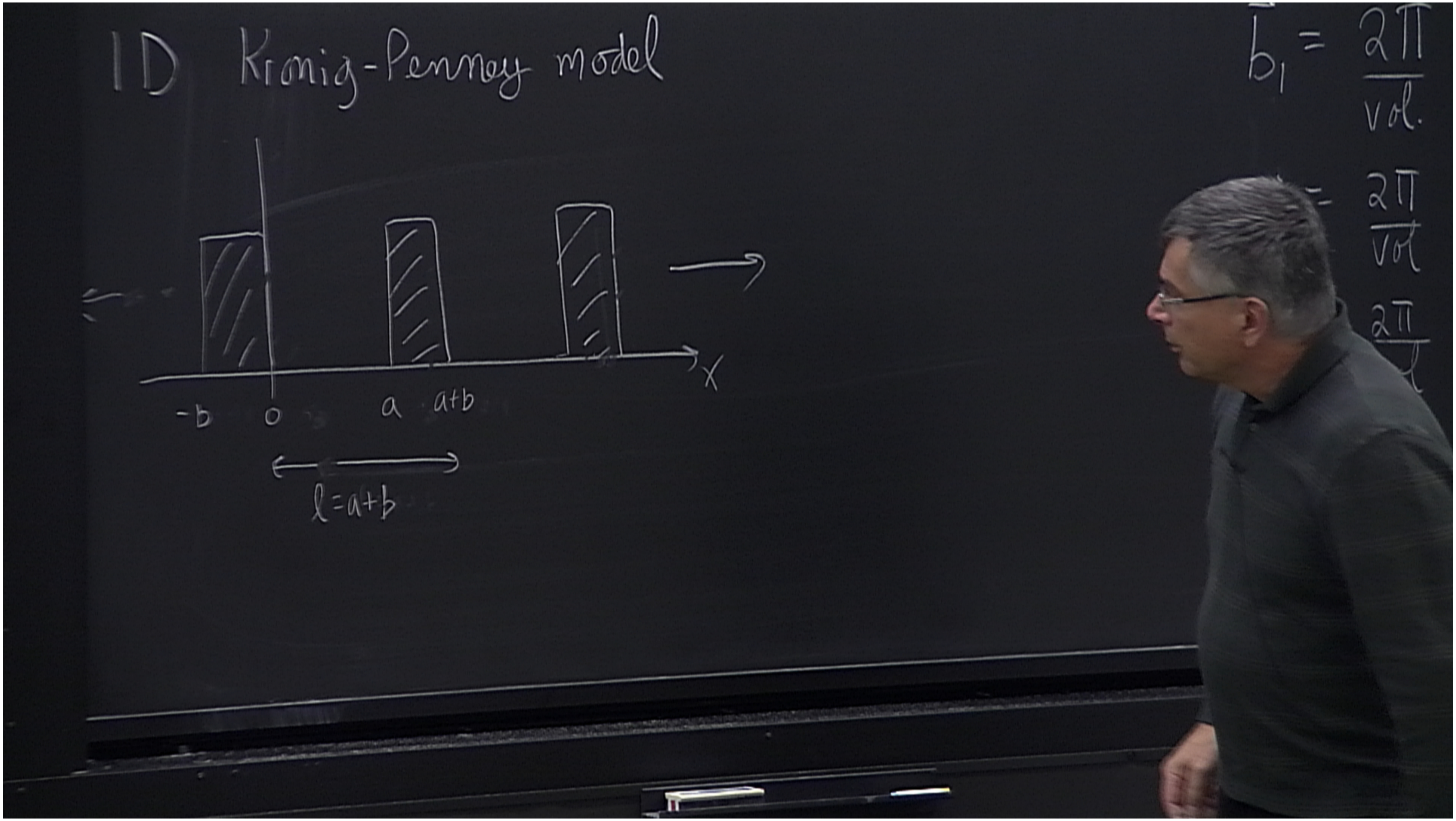
not in the FBZ

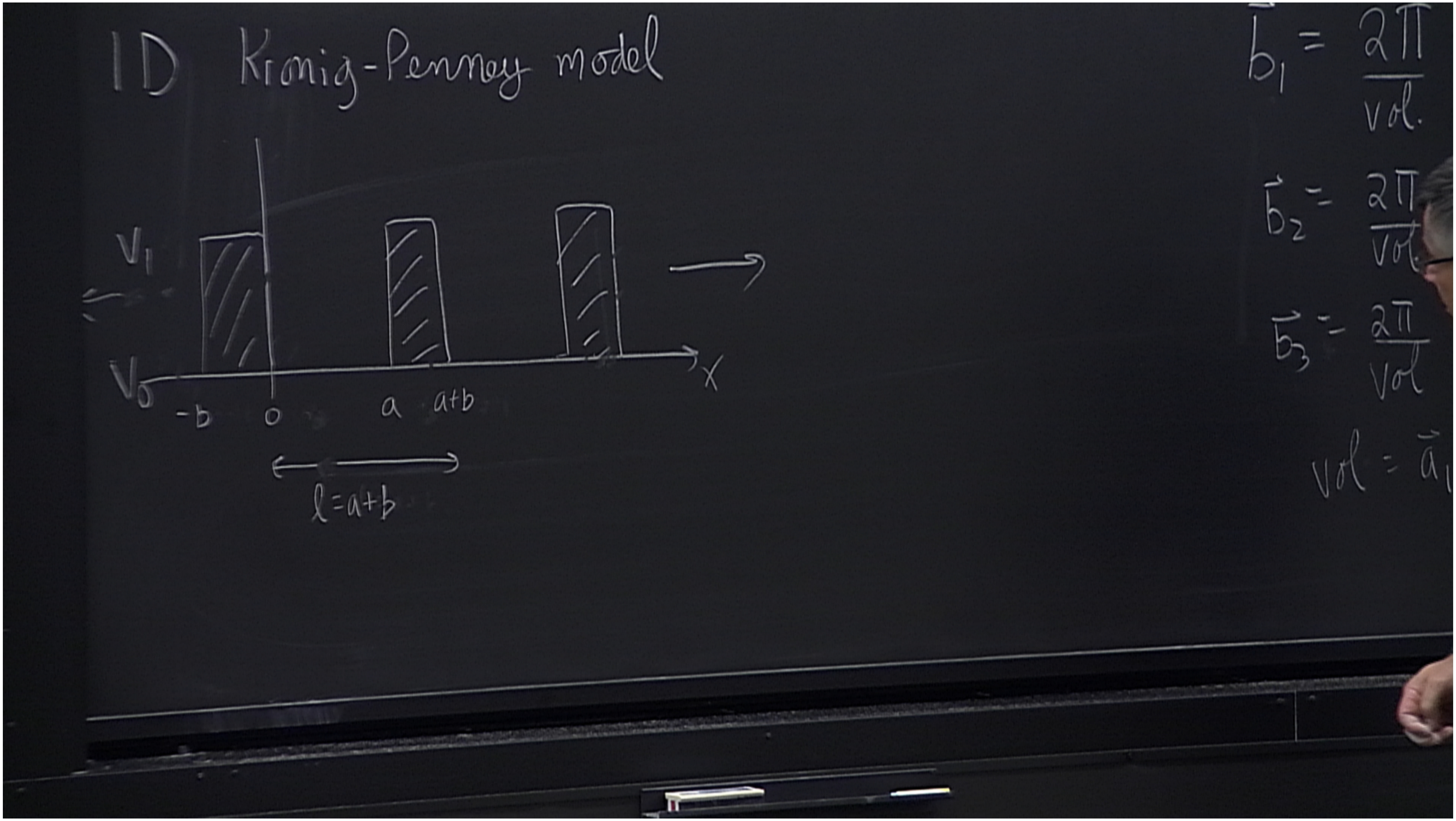
is in the FBZ

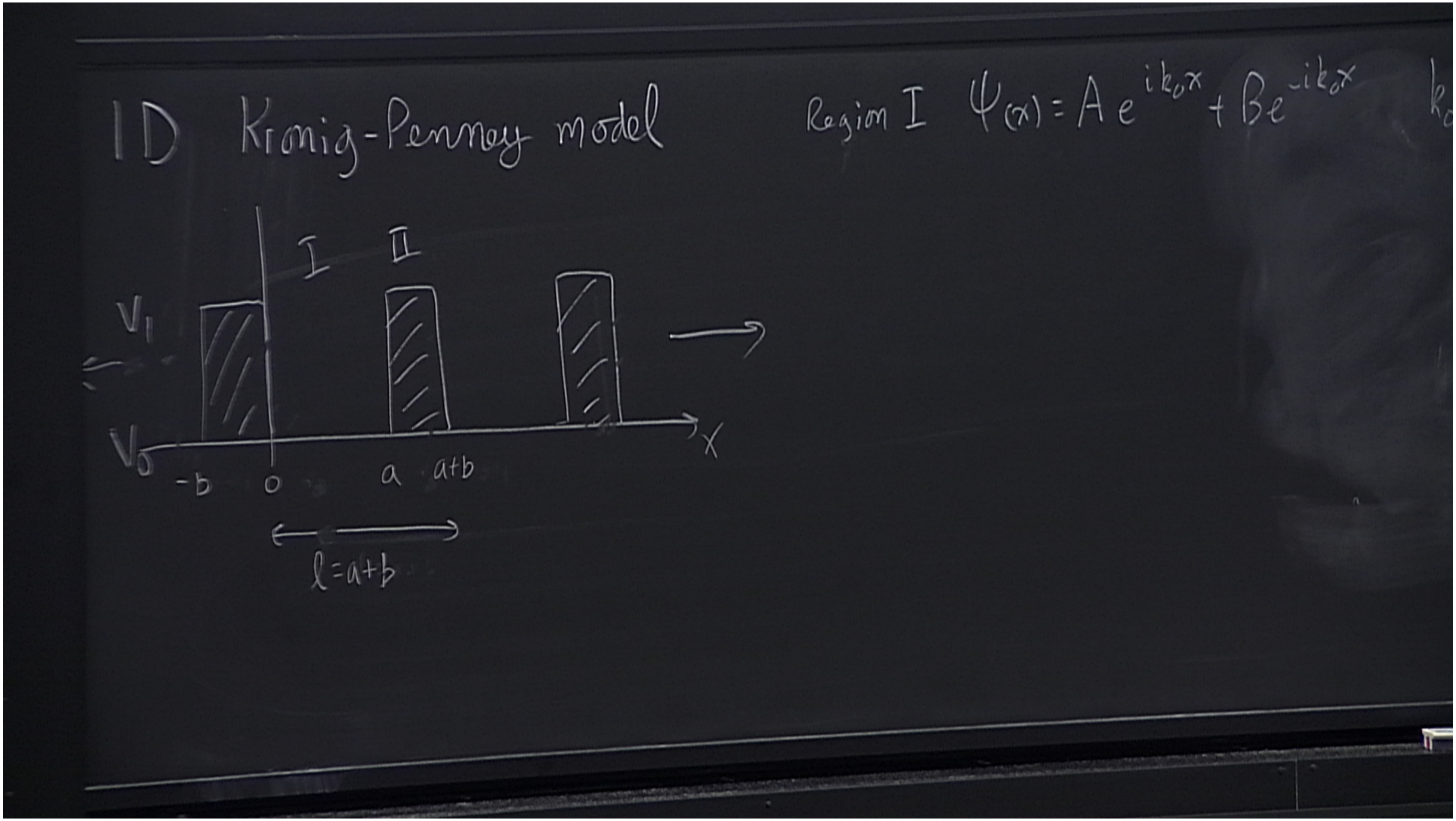


$\psi_{kn}(\vec r+\vec R) = e^{i\vec k\cdot\vec R}\psi_{kn}(\vec r)$
$u(\vec r)$
$\psi_{kn}(\vec r+\vec R) = e^{i\vec k\cdot(\vec r+\vec R)}\,u_{kn}(\vec r+\vec R)$
$u_{kn}(\vec r)$
$= e^{i\vec k\cdot\vec R}\,e^{i\vec k\cdot\vec r}\,u_{kn}(\vec r)$
$\psi_{kn}(\vec r)$
$\vec k' = \vec k + \vec G$
is in the FBZ
not in the FBZ
$\psi_{k'n}(\vec r+\vec R) = e^{ik'\cdot\vec R}\,\psi_{k'n}(\vec r)$
$e^{i(\vec k+\vec G)\cdot\vec R}$

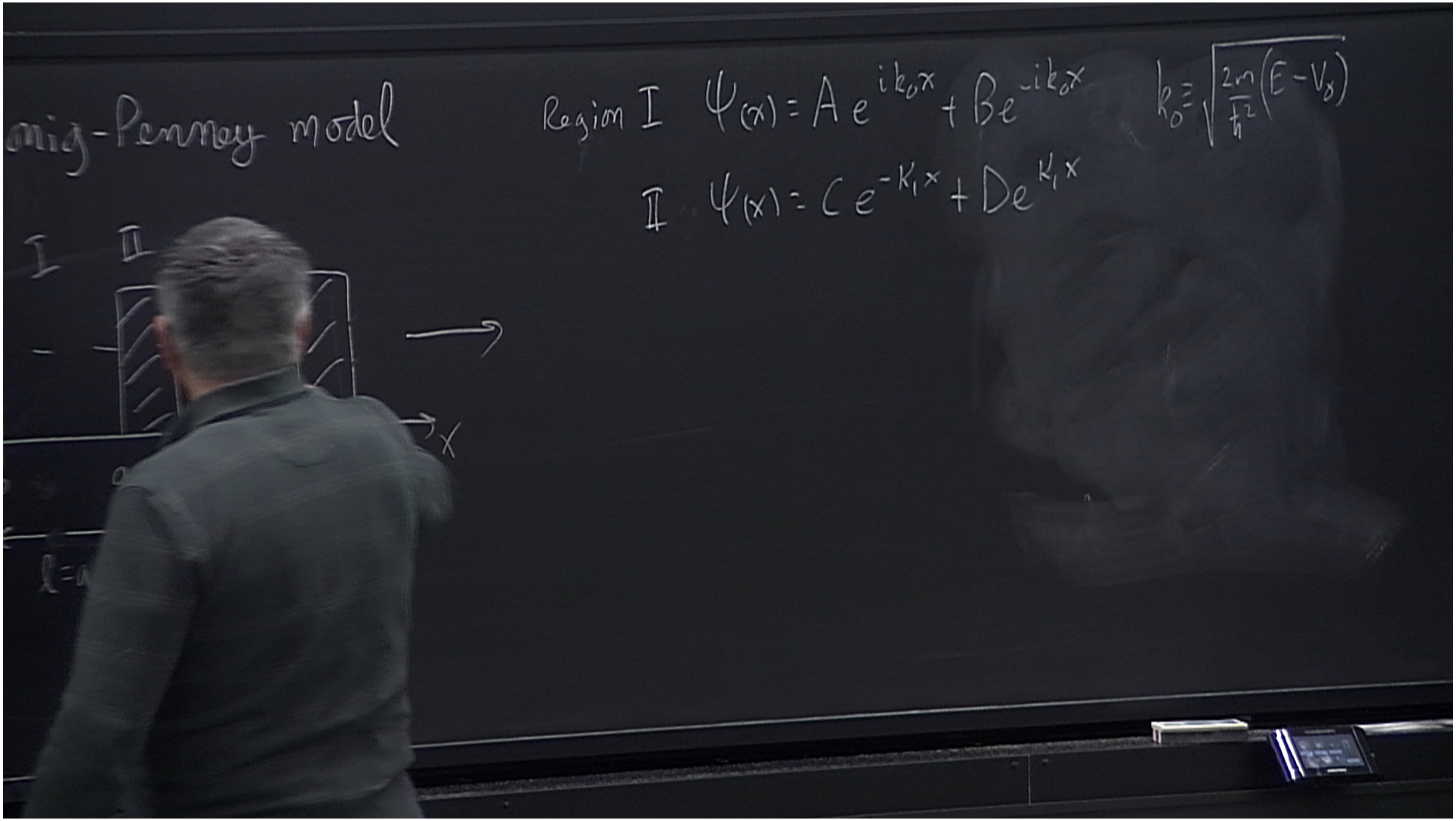

$\vec{k}' = \vec{k} + \vec{G}$
is in the FBZ
not in
$\psi_{k'n}(\vec{r}+\vec{R}) = e^{ik'\cdot\vec{R}}\,\psi_{k'n}(\vec{r})$
$e^{i(\vec{k}+\vec{G})\cdot\vec{R}}$
$e^{i\vec{G}\cdot\vec{R}} = 1$
$\psi_{k'n}(\vec{r}+\vec{R}) = e^{ik\cdot\vec{R}}\,\psi_{k'n}(\vec{r})$

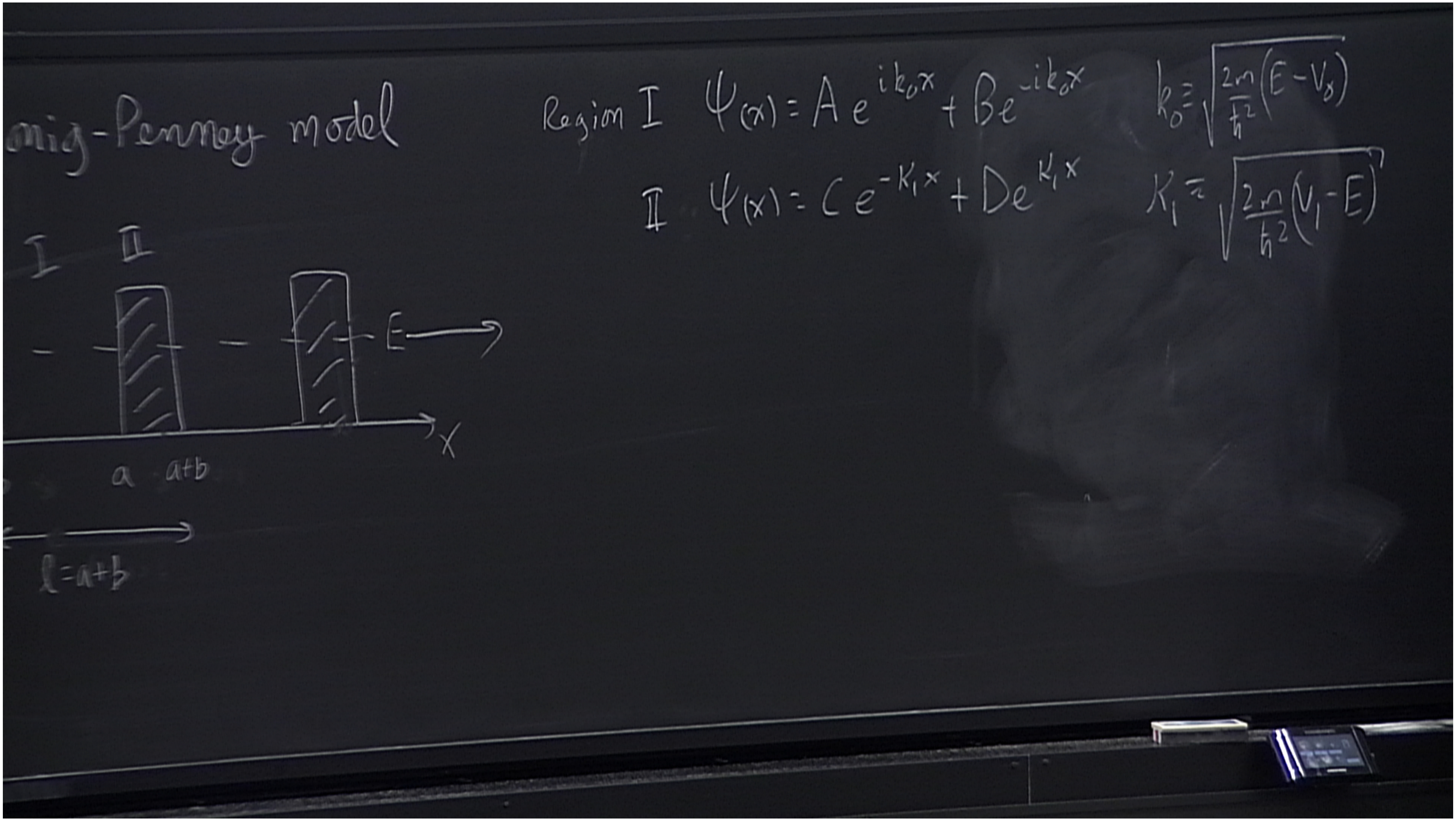

1D Kronig-Penney model
-b
0
a
a+b
x
l=a+b
b1 = 2π / vol.
2π / vol
2π

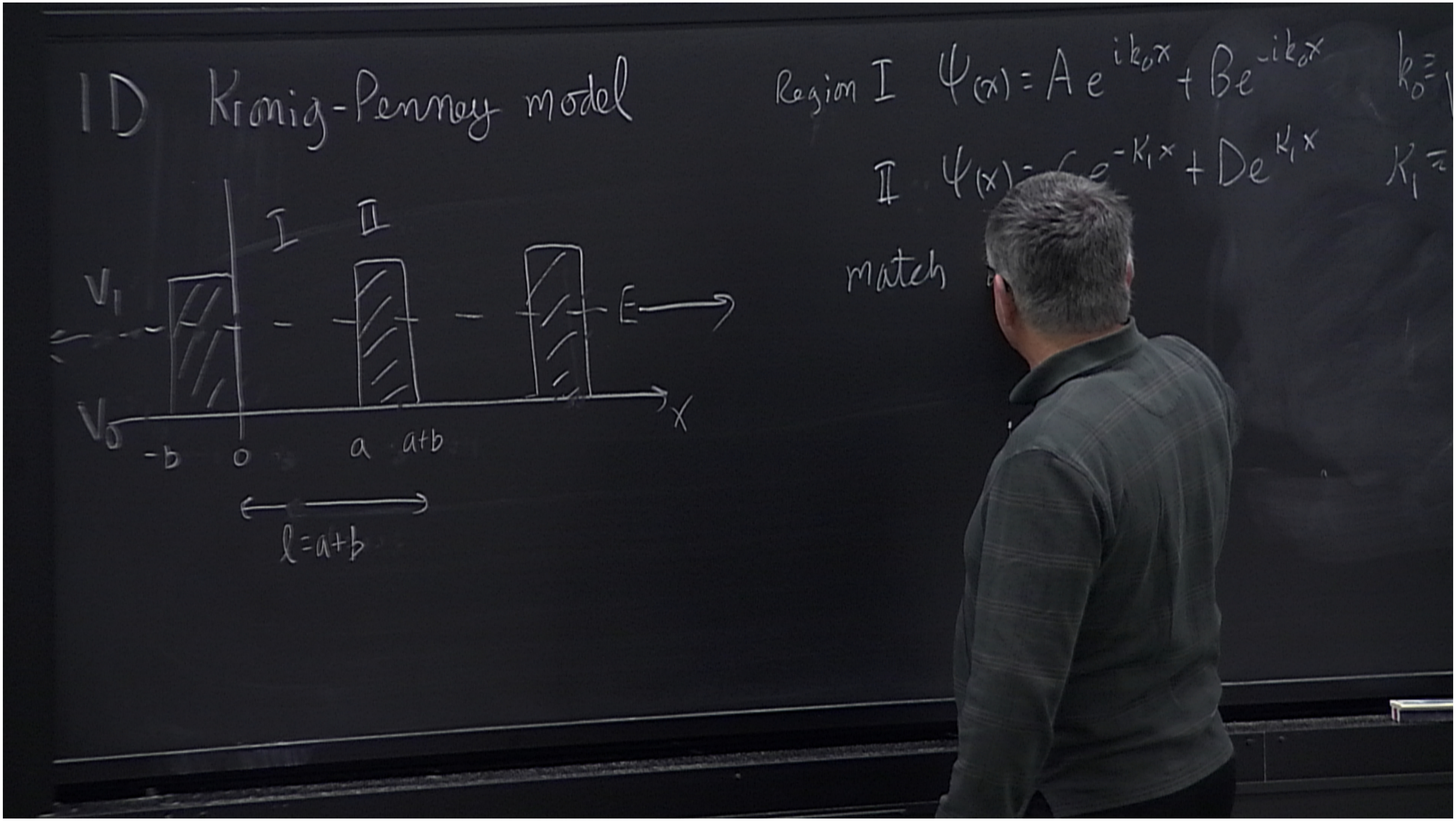

1D Kronig-Penney model
V1
V0
-b
0
a
a+b
x
l=a+b
b1 = 2π / vol.
b2 = 2π / vol.
b3 = 2π / vol
vol = a1

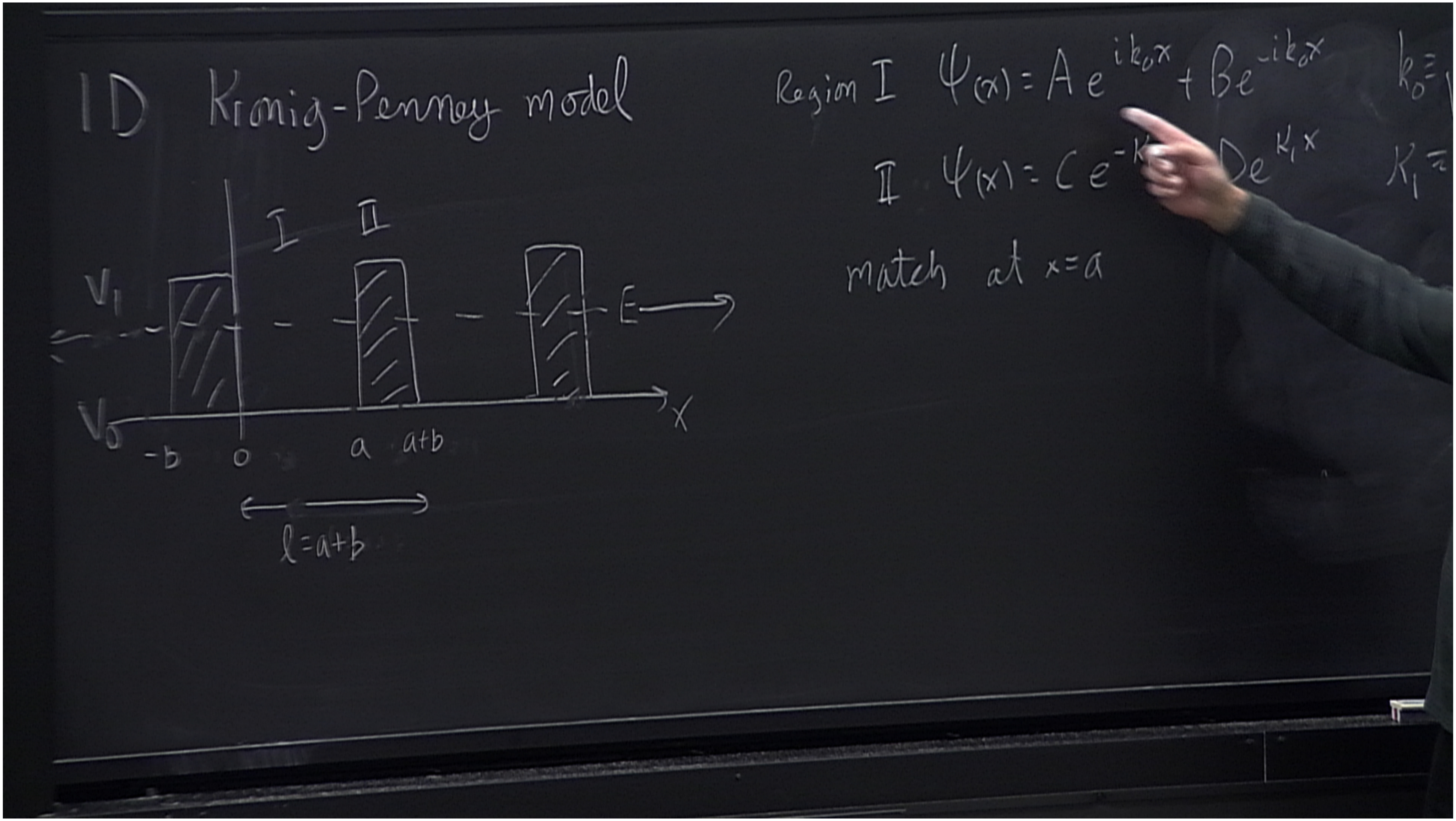


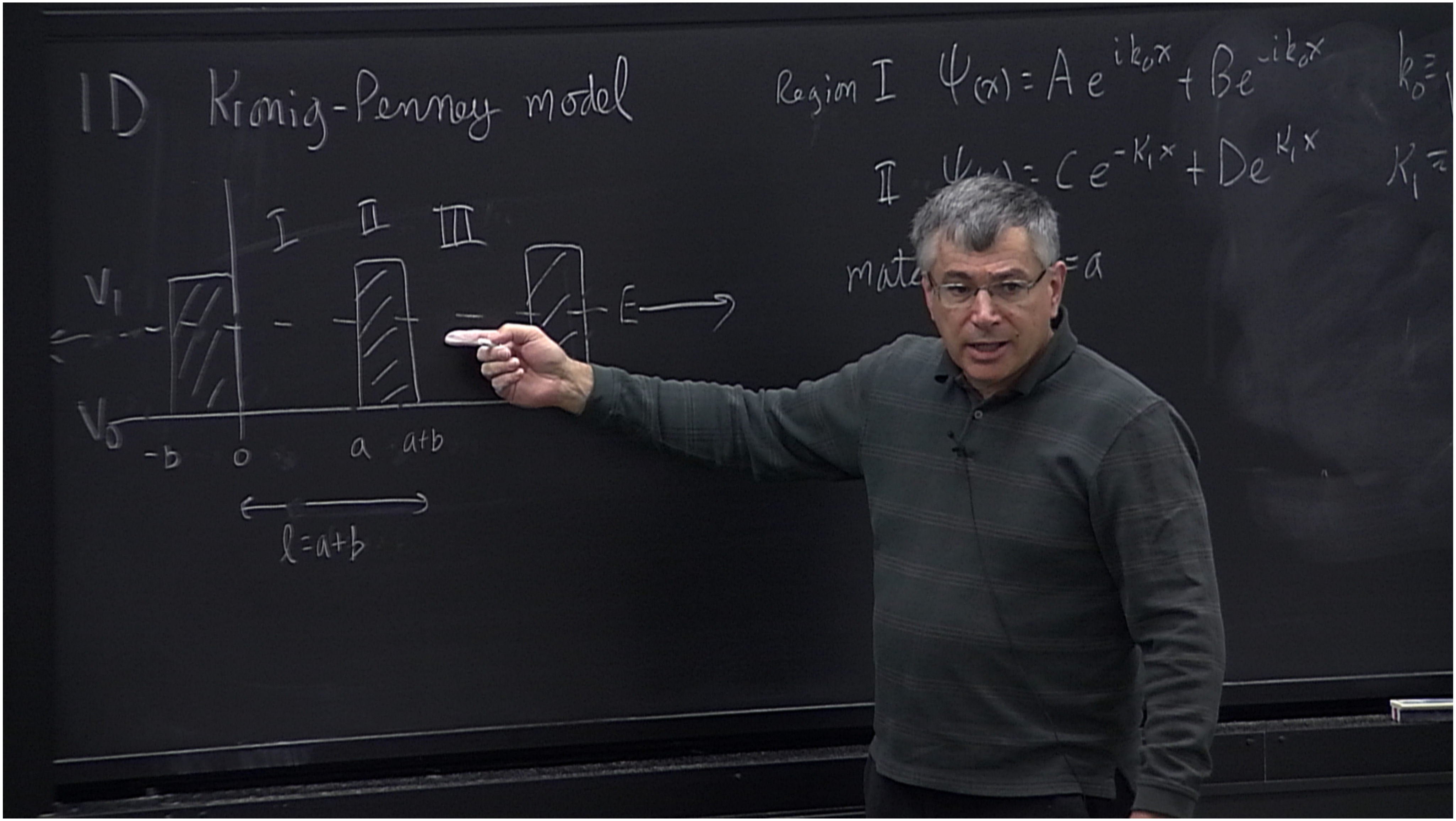
1D Kronig-Penney model
Region I $\psi_{(x)} = A e^{ik_0 x} + B e^{-ik_0 x}$
I
II
V_1
V_0
$-b$
0
a
$a+b$
x
$l = a+b$


nig-Penney model
Region I $\psi(x) = A e^{ik_0 x} + B e^{-ik_0 x}$
$k_0 = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$
II $\psi(x) = C e^{-K_1 x} + D e^{K_1 x}$
I
II
x

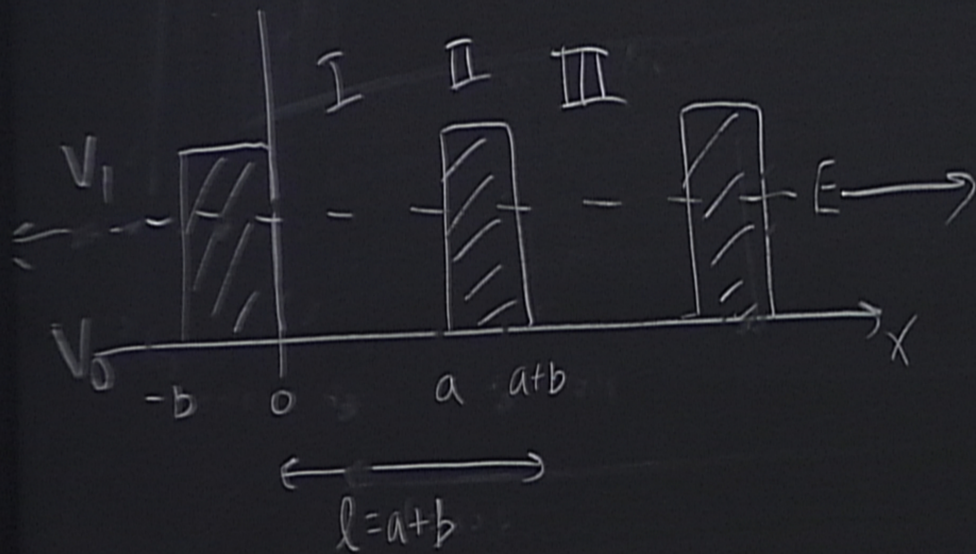

nig-Penney model
Region I $\psi(x) = A e^{ik_0 x} + B e^{-ik_0 x}$
$k_0 = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$
II $\psi(x) = C e^{-K_1 x} + D e^{K_1 x}$
$K_1 = \sqrt{\frac{2m}{\hbar^2}(V_1 - E)}$
I
II
E
x
a
a+b
$l = a+b$


1D Kronig-Penney model
Region I ψ(x) = A e^{ik₀x} + Be^{-ik₀x}
II ψ(x) = Ce^{-K₁x} + De^{K₁x}
match
I
II
V₁
V₀
E
x
-b
0
a
a+b
l=a+b


1D Kronig-Penney model
Region I $\psi(x) = A e^{ik_0 x} + B e^{-ik_0 x}$
$k_0 =$
II $\psi(x) = C e^{-K}$
$D e^{K_1 x}$
$K_1 =$
match at $x=a$
I
II
V_1
V_0
E
x
-b
0
a
a+b
$l = a+b$


1D Kronig-Penney model
Region I ψ(x) = A e^{ik₀x} + B e^{-ik₀x}
II ψ(x) = C e^{-K₁x} + D e^{K₁x}
I
II
III
V₁
V₀
E
-b
0
a
a+b
l=a+b

1D Kronig-Penney model



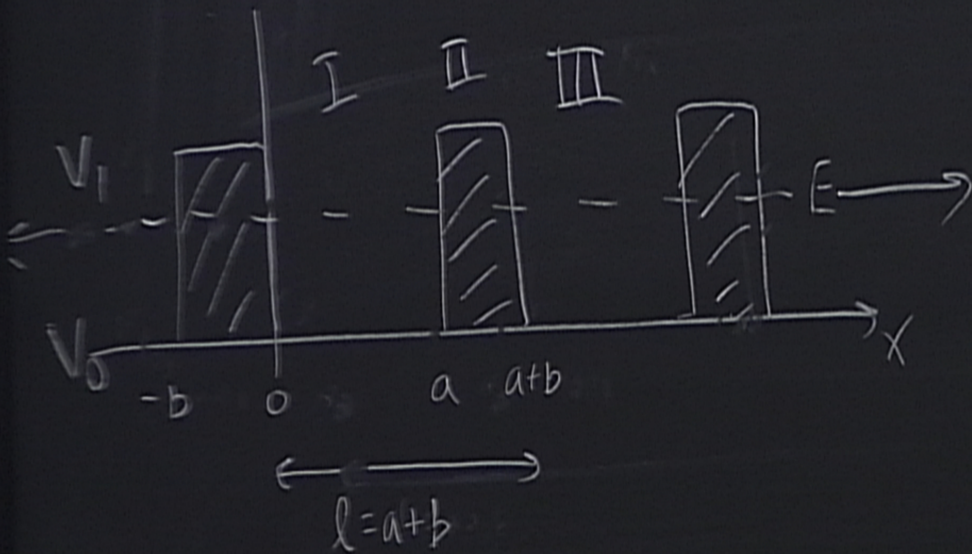
Region I $\psi(x) = A e^{ik_0 x} + B e^{-ik_0 x}$ $k_0 =$

II $\psi(x) = C e^{-K_1 x} + D e^{K_1 x}$ $K_1 =$

match at $x = a$

$$\psi(x+l) = e^{ik \cdot l}\,\psi(x)$$

1D Kronig-Penney model



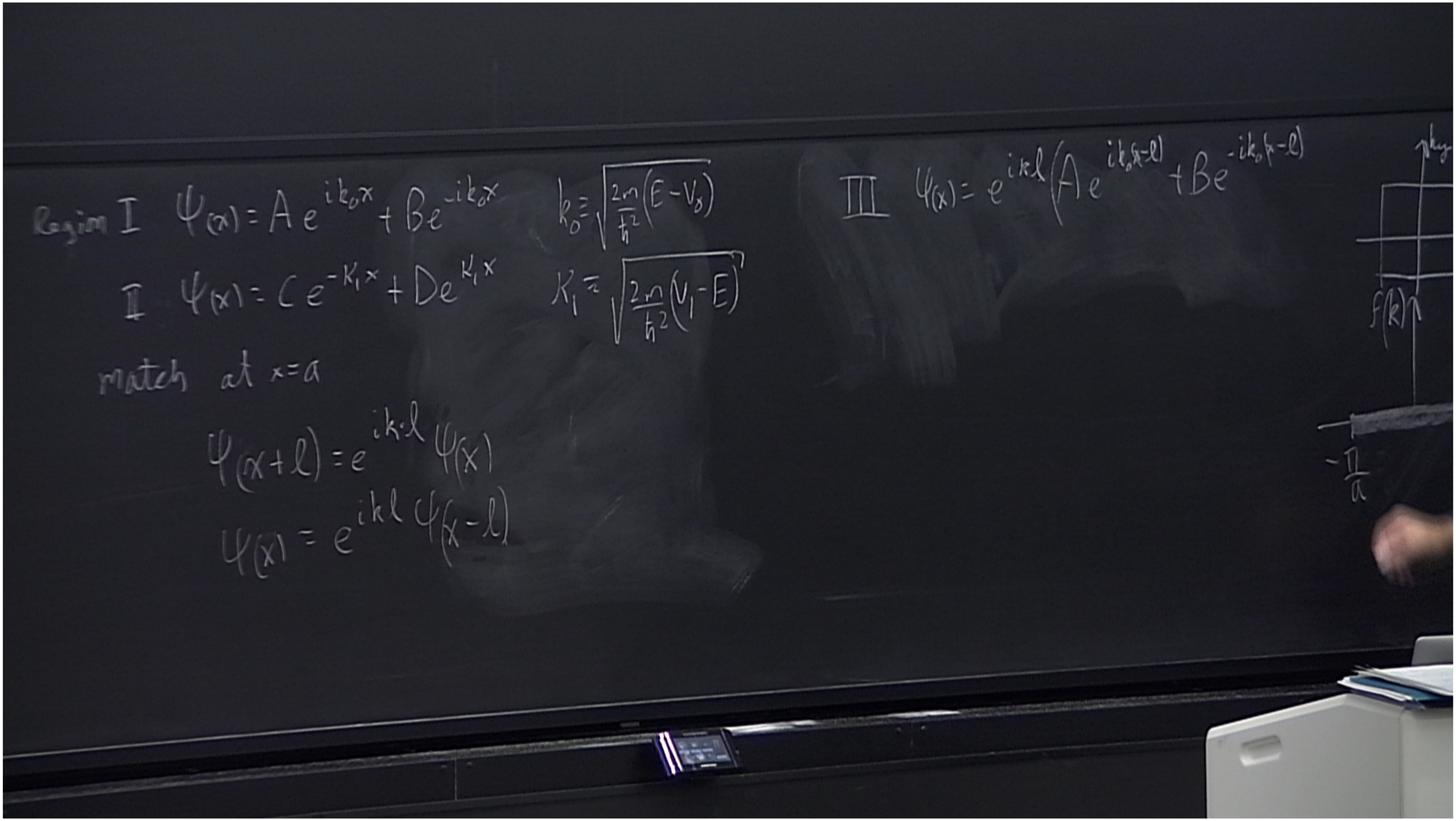
Region I $\psi(x) = A e^{ik_0 x} + B e^{-ik_0 x}$ $k_0 =$

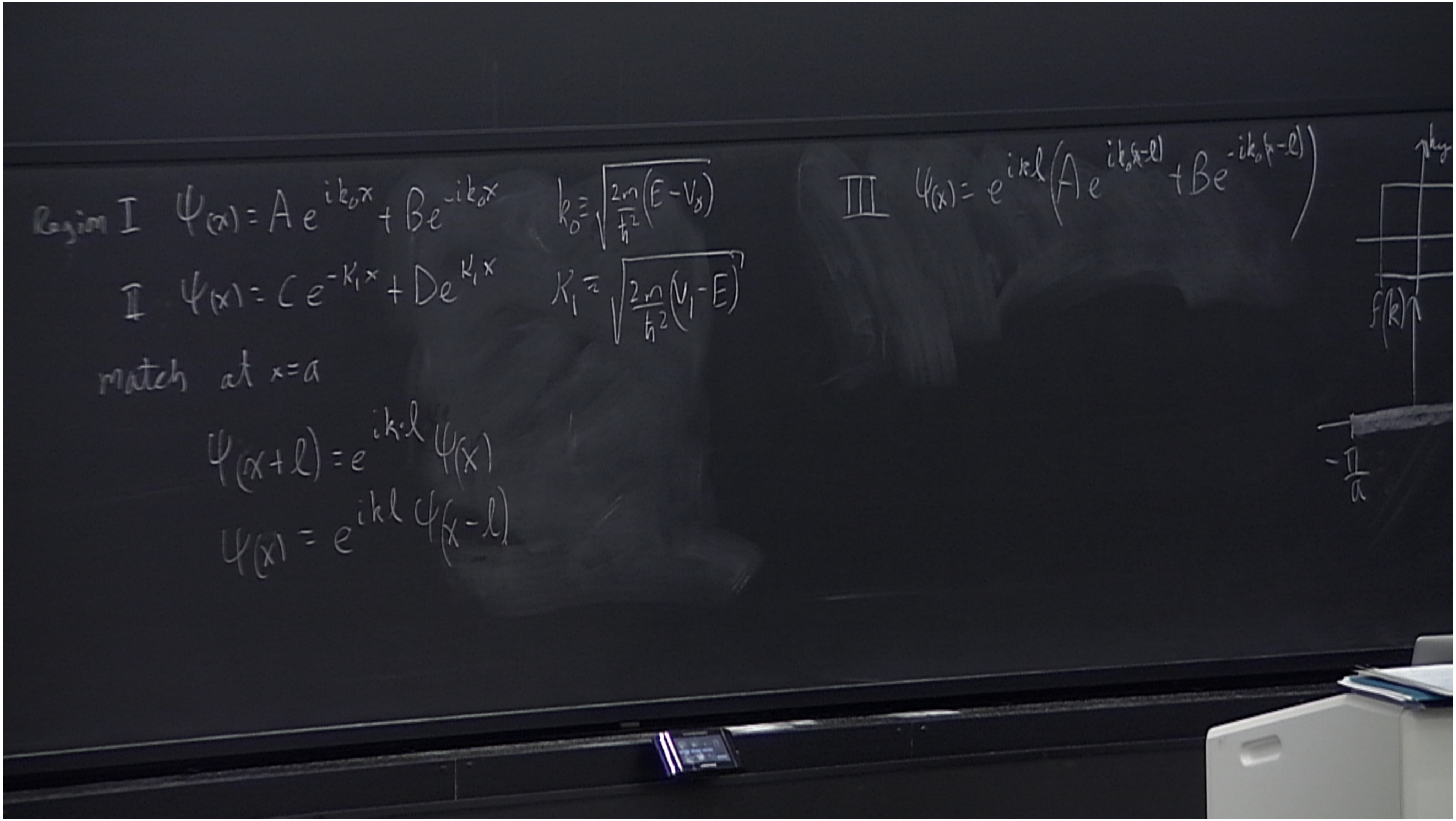
II $\psi(x) = C e^{-K_1 x} + D e^{K_1 x}$ $K_1 =$

match at $x = a$

$$\psi(x+l) = e^{ik \cdot l}\, \psi(x)$$

$$\psi(x) = e^{ikl}\, \psi(x-l)$$


Region I $\psi(x) = Ae^{ik_0x} + Be^{-ik_0x}$
$k_0 \equiv \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$
II $\psi(x) = Ce^{-K_1x} + De^{K_1x}$
$K_1 = \sqrt{\frac{2m}{\hbar^2}(V_1 - E)}$
match at $x=a$
$\psi(x+l) = e^{ik\cdot l}\psi(x)$
$\psi(x) = e^{ikl}\psi(x-l)$
III $\psi(x) = e^{ikl}\left(Ae^{ik_0(x-l)} + Be^{-ik_0(x-l)}\right)$
$f(k)$
$-\frac{\pi}{a}$


Region I $\psi(x) = Ae^{ik_0x} + Be^{-ik_0x}$
$k_0 \equiv \sqrt{\frac{2m}{\hbar^2}(E-V_0)}$
II $\psi(x) = Ce^{-K_1x} + De^{K_1x}$
$K_1 = \sqrt{\frac{2m}{\hbar^2}(V_1-E)}$
match at $x=a$
$\psi(x+l) = e^{ik\cdot l}\psi(x)$
$\psi(x) = e^{ikl}\psi(x-l)$
III $\psi(x) = e^{ikl}\left(Ae^{ik_0(x-l)} + Be^{-ik_0(x-l)}\right)$
$f(k)$
$-\frac{\pi}{a}$

Region I $\psi(x) = A e^{ik_0 x} + B e^{-ik_0 x}$ $k_0 \equiv \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$

II $\psi(x) = C e^{-K_1 x} + D e^{K_1 x}$ $K_1 = \sqrt{\frac{2m}{\hbar^2}(V_1 - E)}$

match at $x = a$

$$\psi(x + l) = e^{ik \cdot l}\psi(x)$$

$$\psi(x) = e^{ikl}\psi(x - l)$$

III $\psi(x) = e^{ikl}\left(A e^{ik_0(x-l)} + B e^{-ik_0(x-l)}\right)$

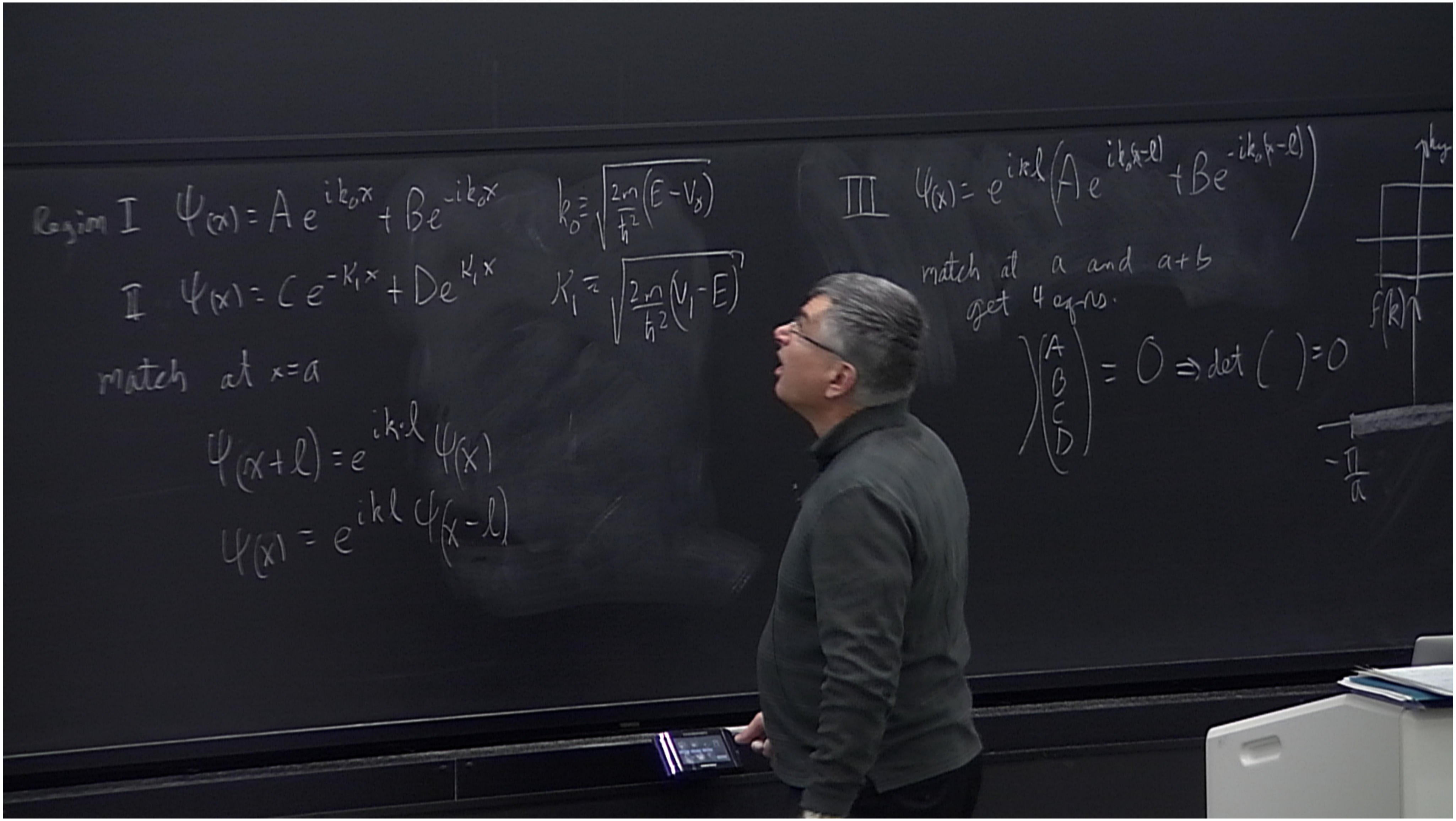
match at a and $a+b$

get 4 eqns.

$$\begin{pmatrix} & & & \\ & & & \\ & & & \\ & & & \end{pmatrix}\begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = 0$$

$f(k)$

$-\frac{\pi}{a}$


Region I ψ(x) = A e^{ik₀x} + B e^{-ik₀x}
k₀ ≡ √(2m/ħ² (E − V₀))
II ψ(x) = C e^{-K₁x} + D e^{K₁x}
K₁ ≡ √(2m/ħ² (V₁ − E))
match at x=a
ψ(x+l) = e^{ik·l} ψ(x)
ψ(x) = e^{ikl} ψ(x−l)
III ψ(x) = e^{ikl}(A e^{ik₀(x−l)} + B e^{-ik₀(x−l)})
match at a and a+b
get 4 eq-ns.
(A B C D) = 0 ⇒ det ( ) = 0
f(k)
−π/a

$$\cos kl = \cosh K_1 b \cos k_0 a + \frac{K_1^2 - k_0^2}{2K_1 k_0} \sinh K_1 b \sin k_0 a \qquad E < V_1$$

$$\cos kl = \cosh K_1 b \cos k_0 a + \frac{K_1^2 - k_0^2}{2K_1 k_0} \sinh K_1 b \sin k_0 a \qquad E < V_1$$

$$\cos kl = \cos k_1 b \cos k_0 a - \frac{k_1^2 + k_0^2}{2k_1 k_0} \sin k_1 b \sin k_0 a \qquad E > V_1 \quad K_1 = i k_1$$

$$\cos kl = \cosh K_1 b \cos k_0 a + \frac{K_1^2 - k_0^2}{2 K_1 k_0} \sinh K_1 b \sin k_0 a \qquad E < V_1$$

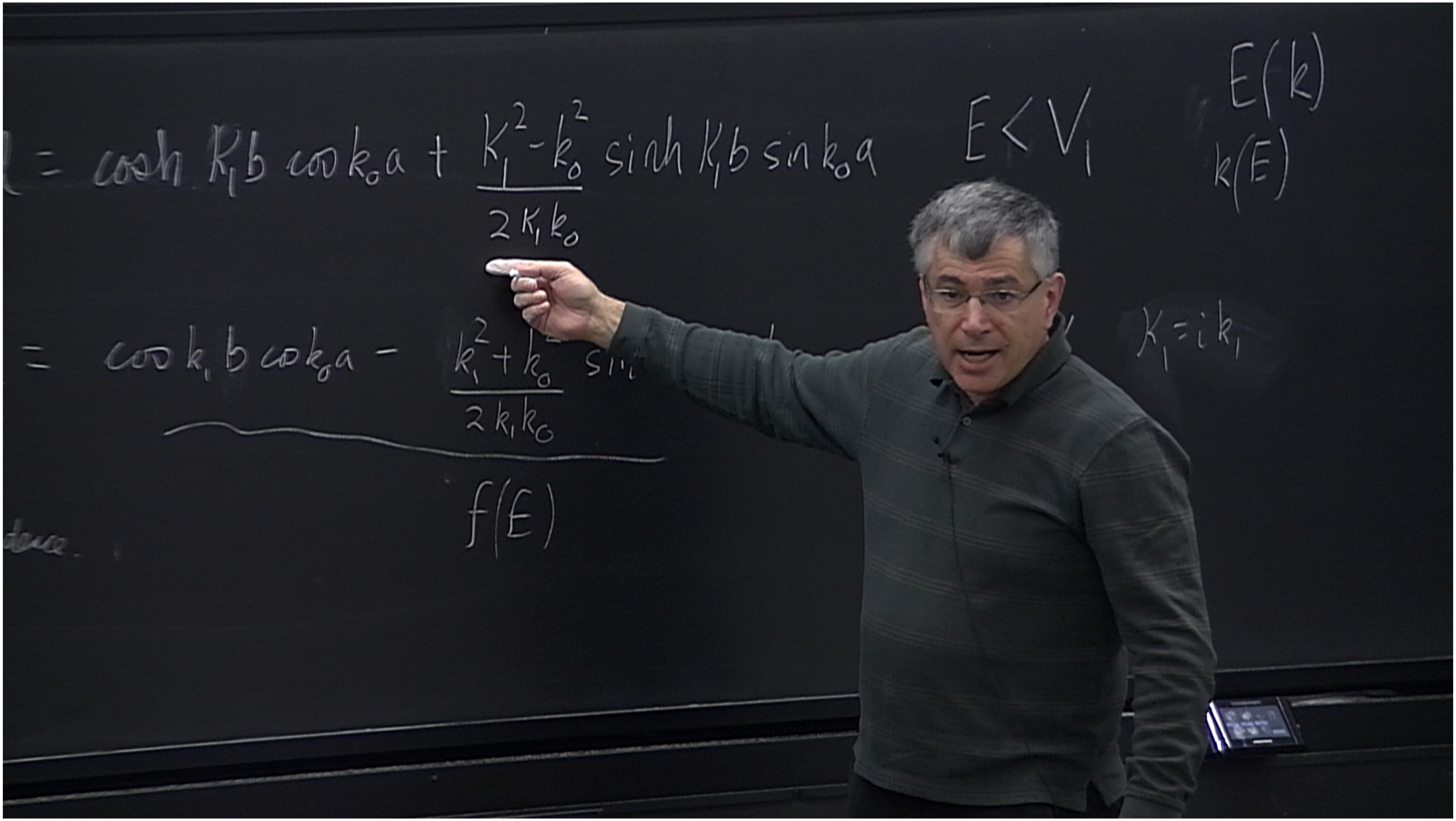
$$\cos kl = \cos k_1 b \cos k_0 a - \frac{k_1^2 + k_0^2}{2 k_1 k_0} \sin k_1 b \sin k_0 a \qquad E > V_1 \qquad K_1 = i k_1$$

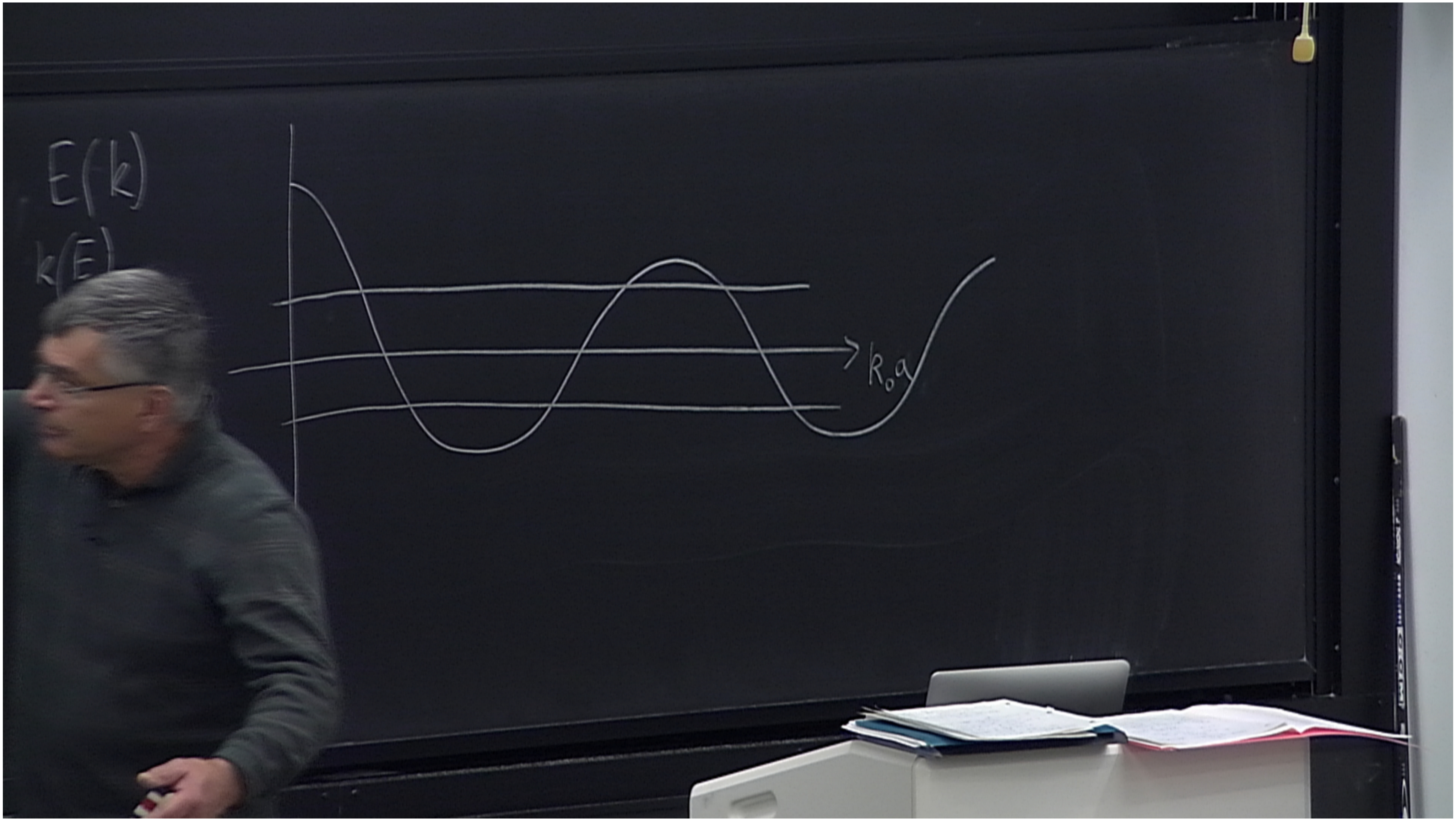
only k dependence.

$$\cos kl = \cosh K_1 b \cos k_0 a + \frac{K_1^2 - k_0^2}{2K_1 k_0} \sinh K_1 b \sin k_0 a \qquad E < V_1$$

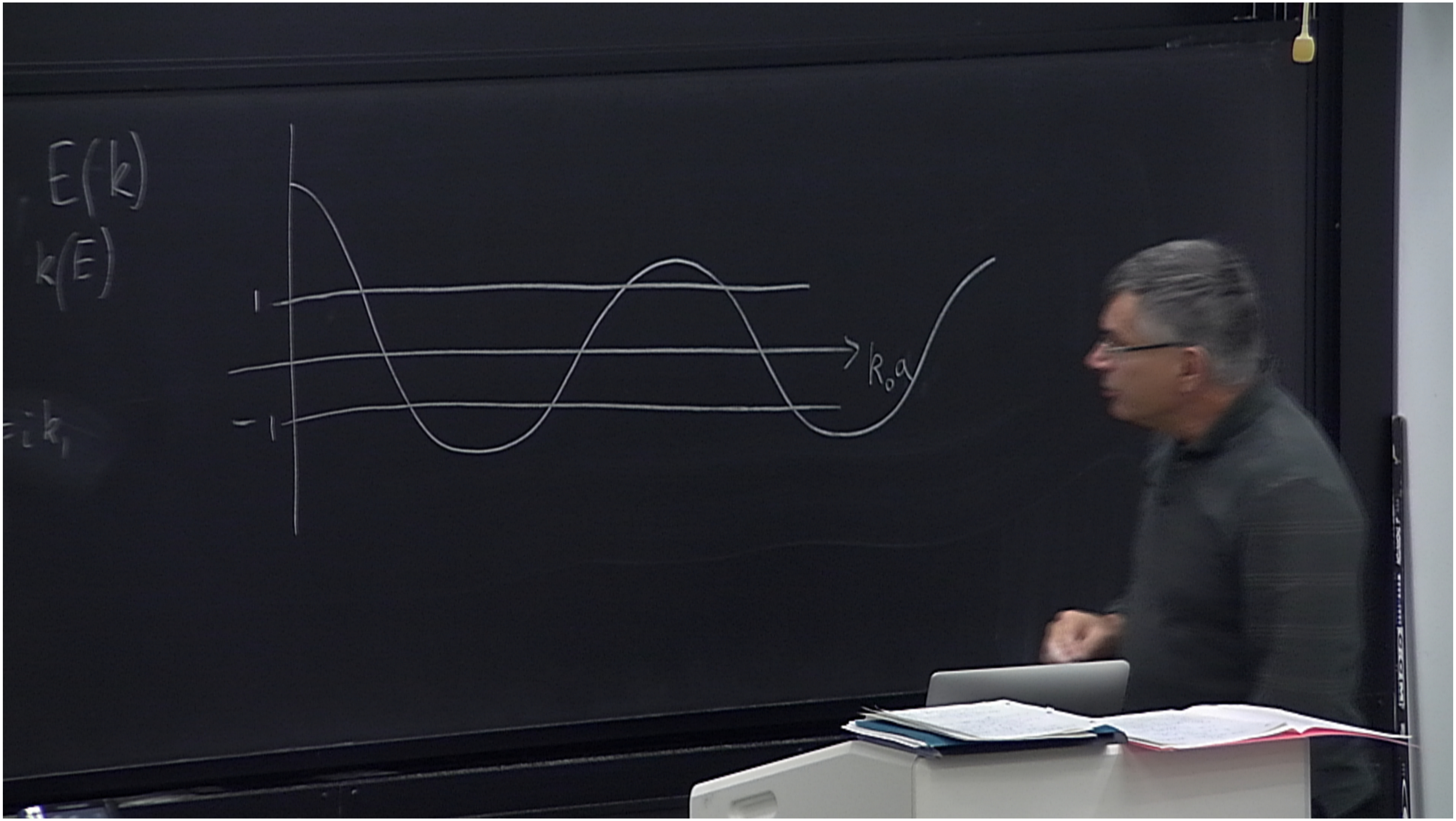
$$\cos kl = \underbrace{\cos k_1 b \cos k_0 a - \frac{k_1^2 + k_0^2}{2k_1 k_0} \sin k_1 b \sin k_0 a}_{f(E)} \qquad E > V_1 \quad K_1 = i k_1$$

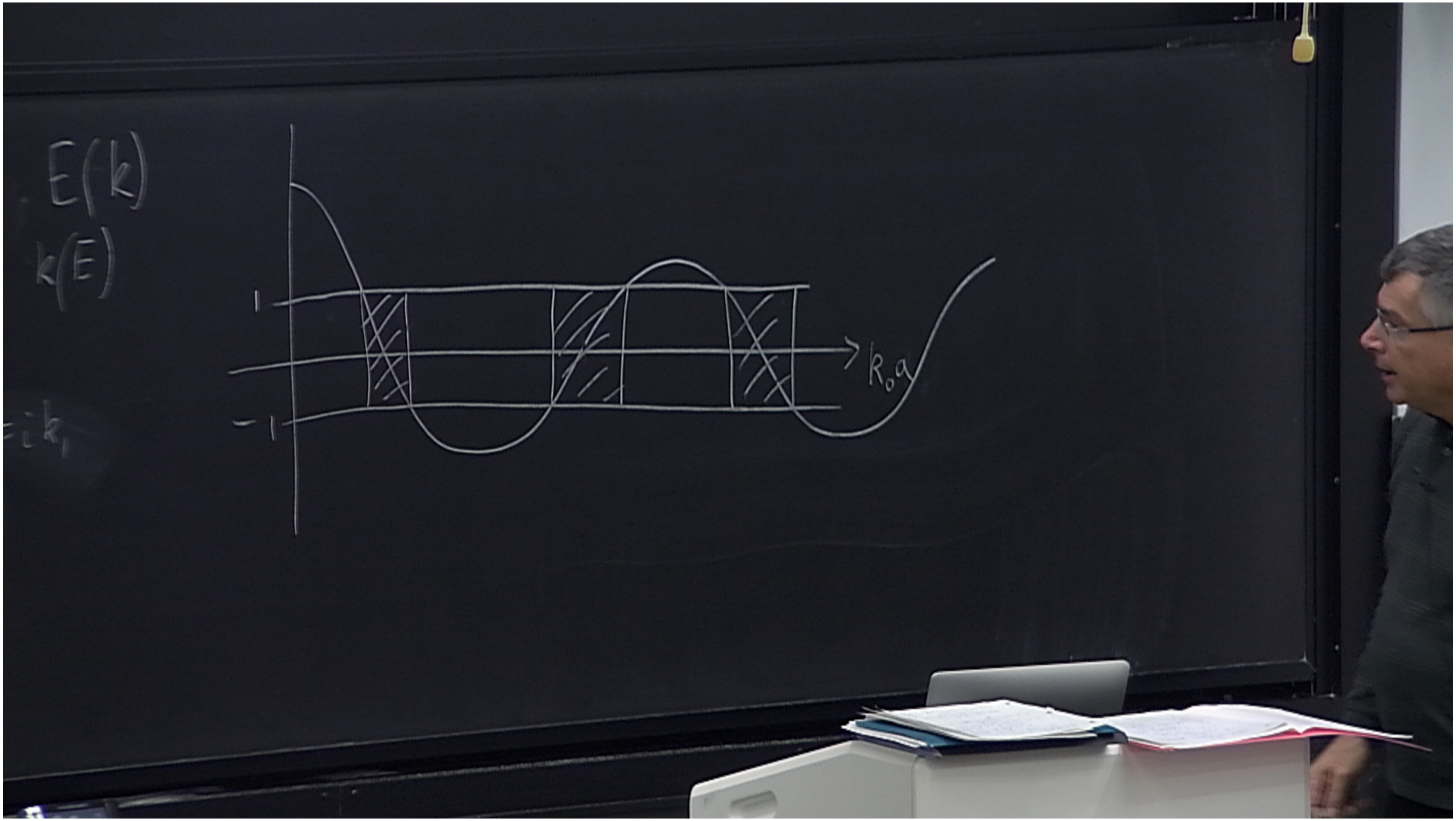
only k dependence.

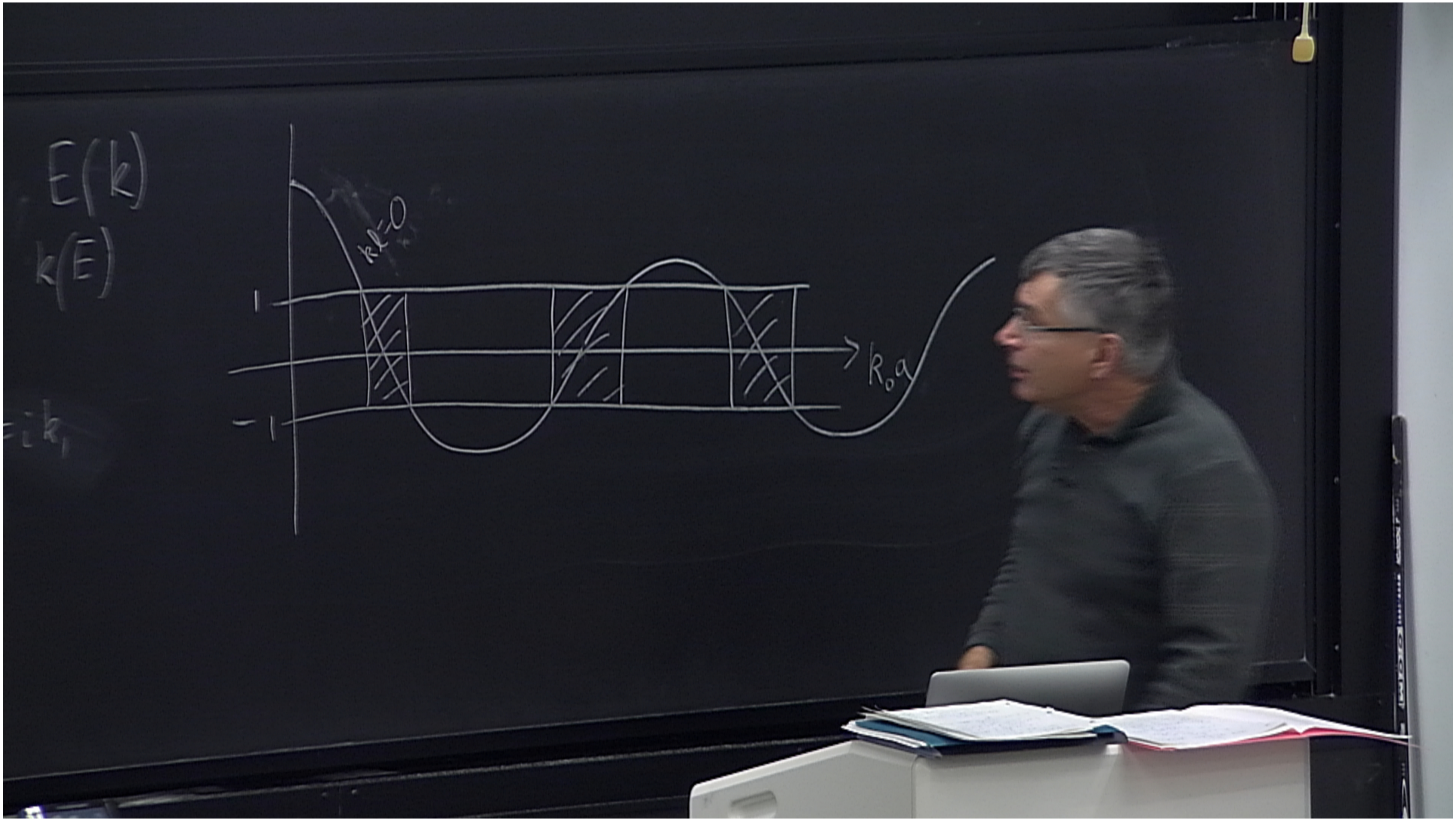

= cosh K1b cos k0a + (K1^2 - k0^2)/(2K1k0) sinh K1b sin k0a
E < V1
E(k)
k(E)
= cos k1b cos k0a - (k1^2 + k0^2)/(2k1k0)
K1 = ik1
f(E)

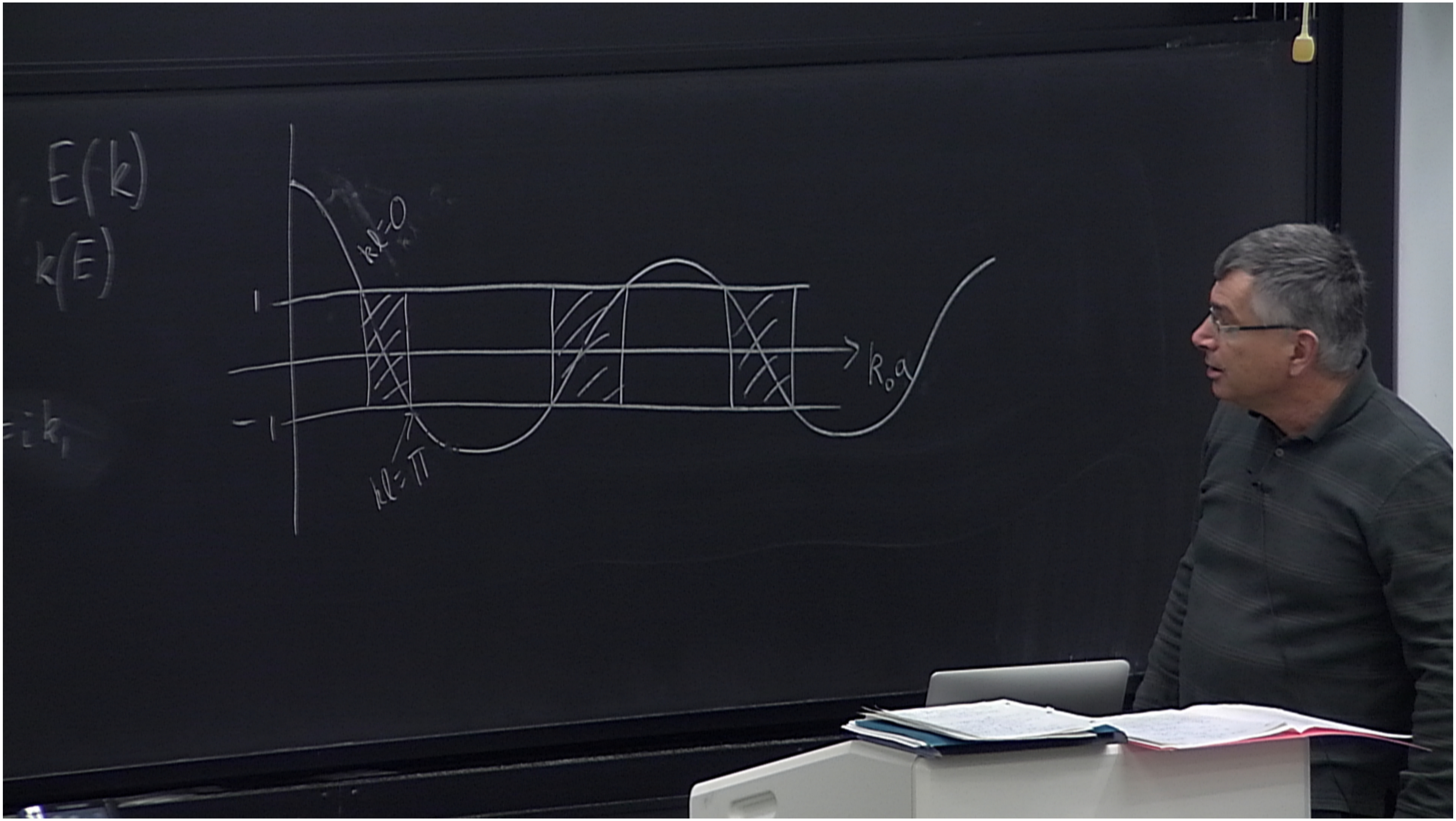


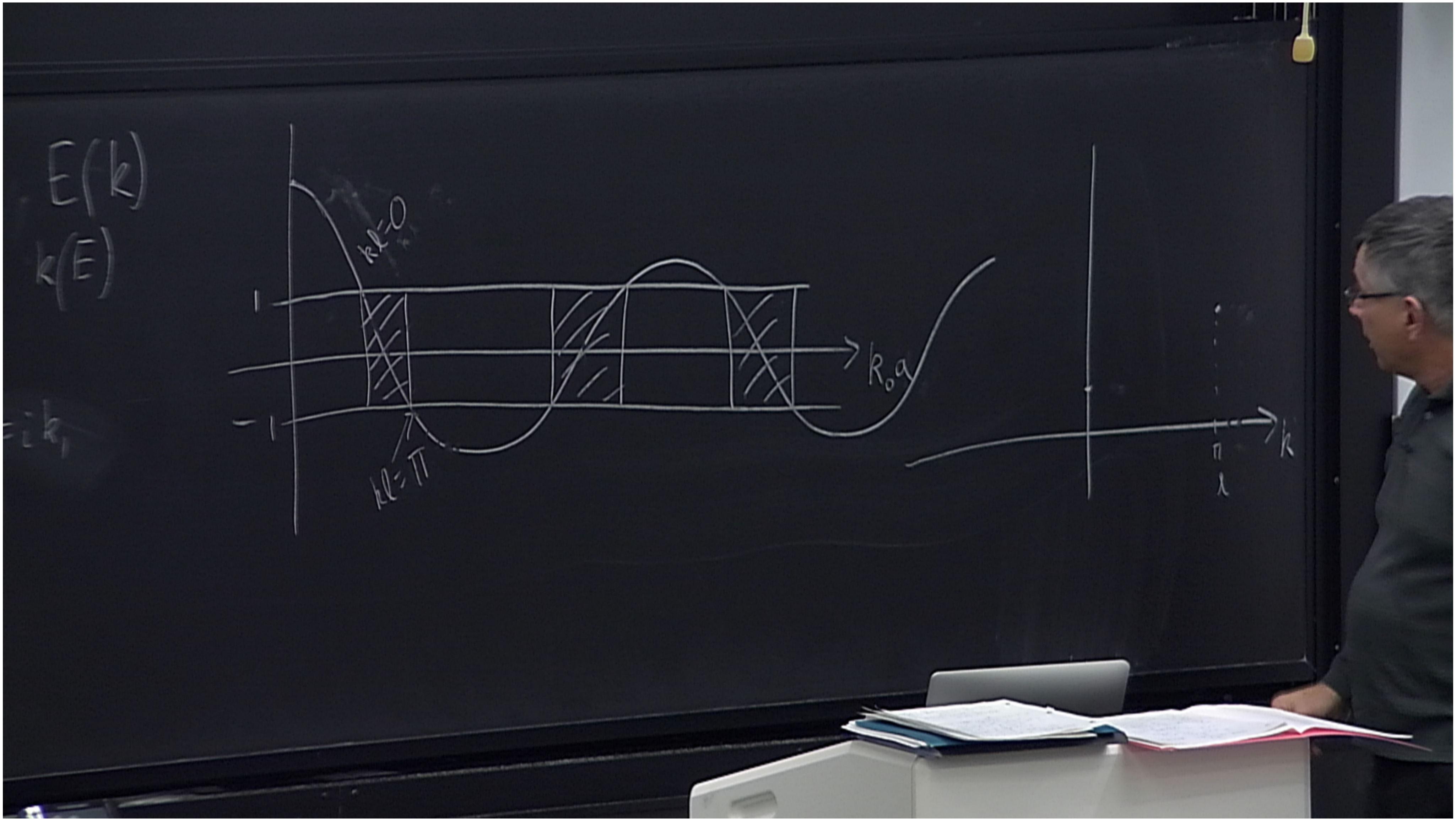
E(k)
k(E)
$k_0 a$


E(k)
k(E)
1
-1
k₀a

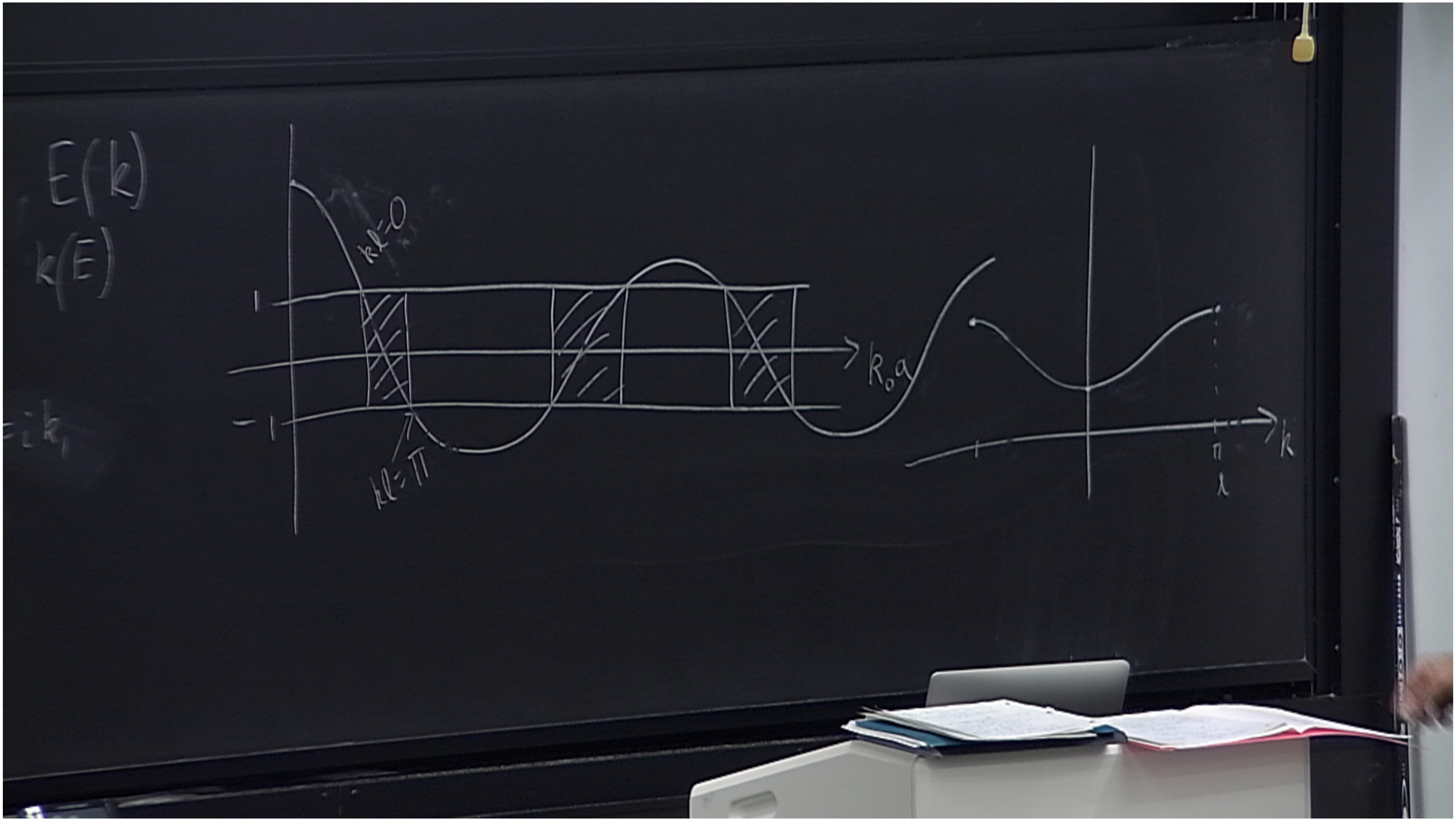

E(k)
k(E)
1
-1
$k_0 a$

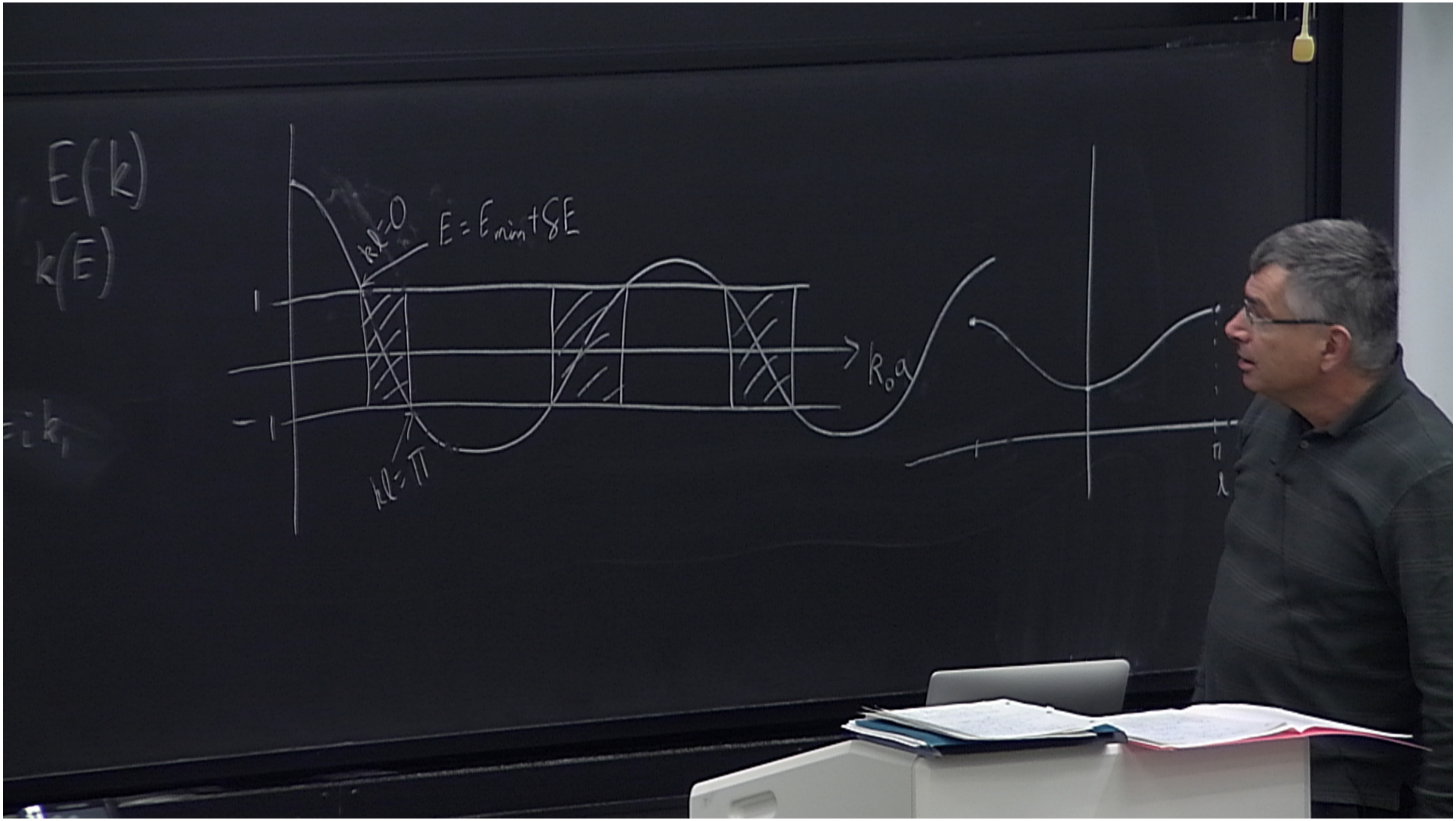

E(k)
k(E)
1
-1
k₀a

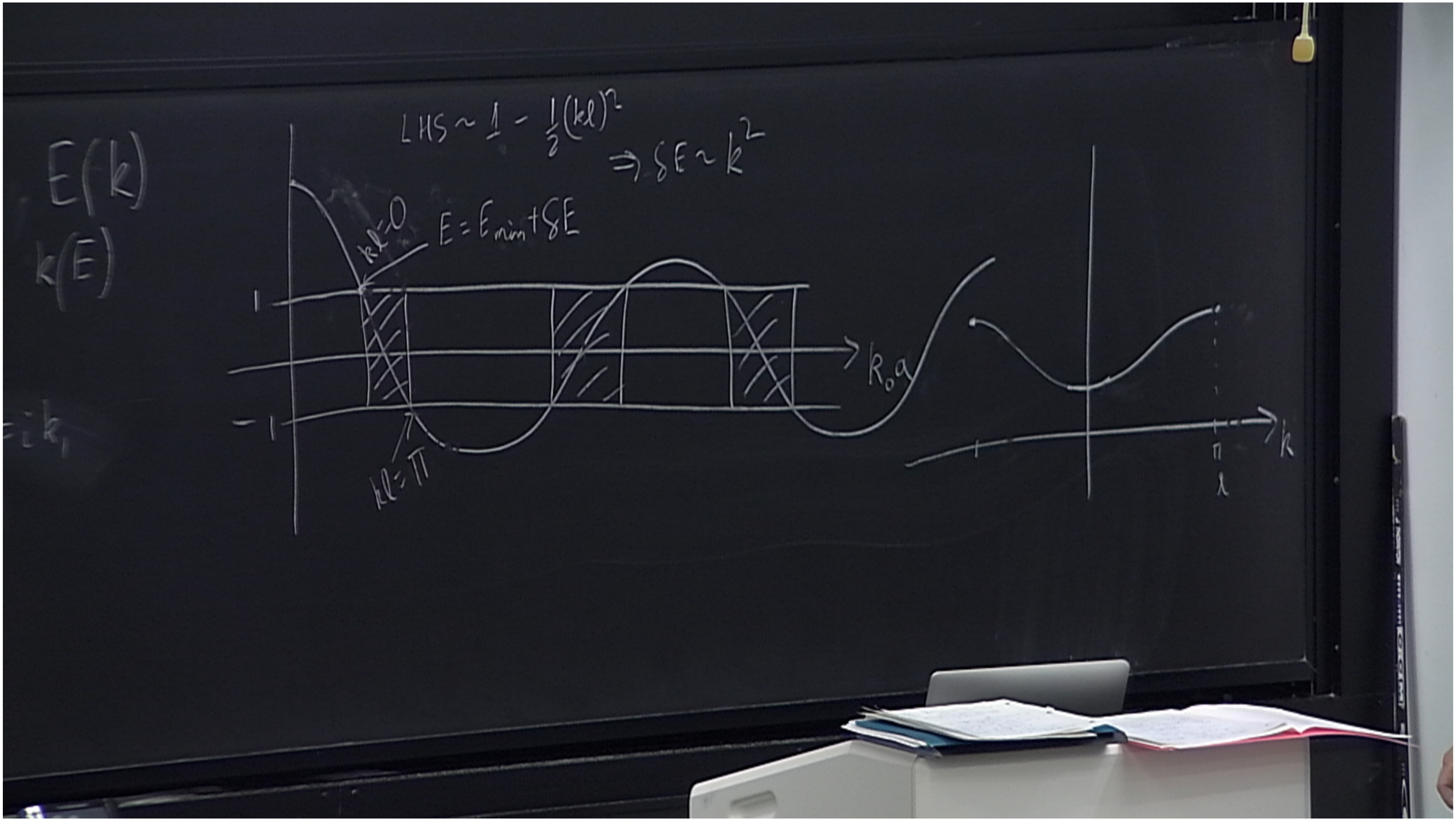

E(k)
k(E)
kl=0
kl=π
1
-1
$k_0 a$

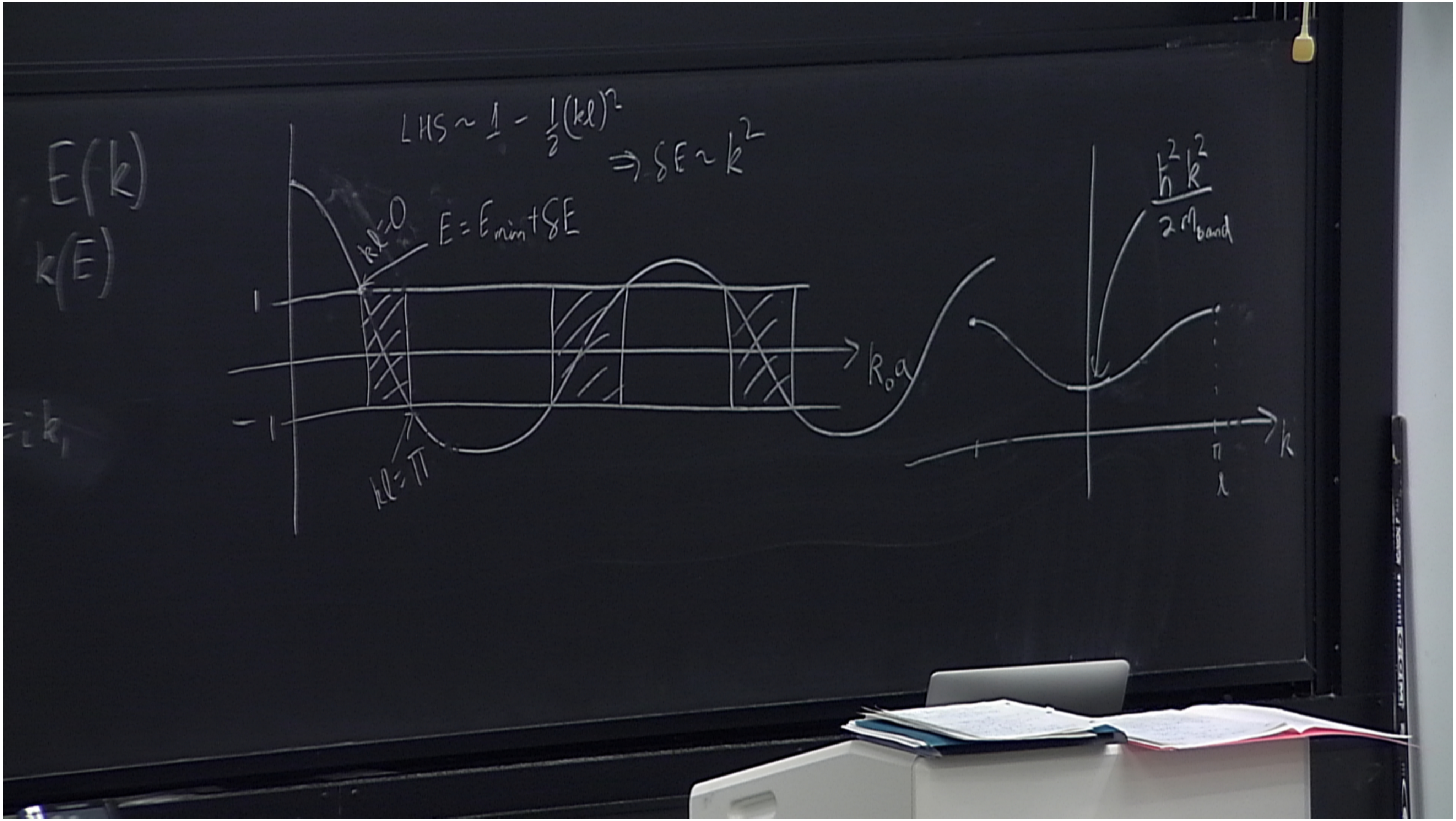


E(k)
k(E)
kℓ=0
kℓ=π
k₀a
1
−1
k

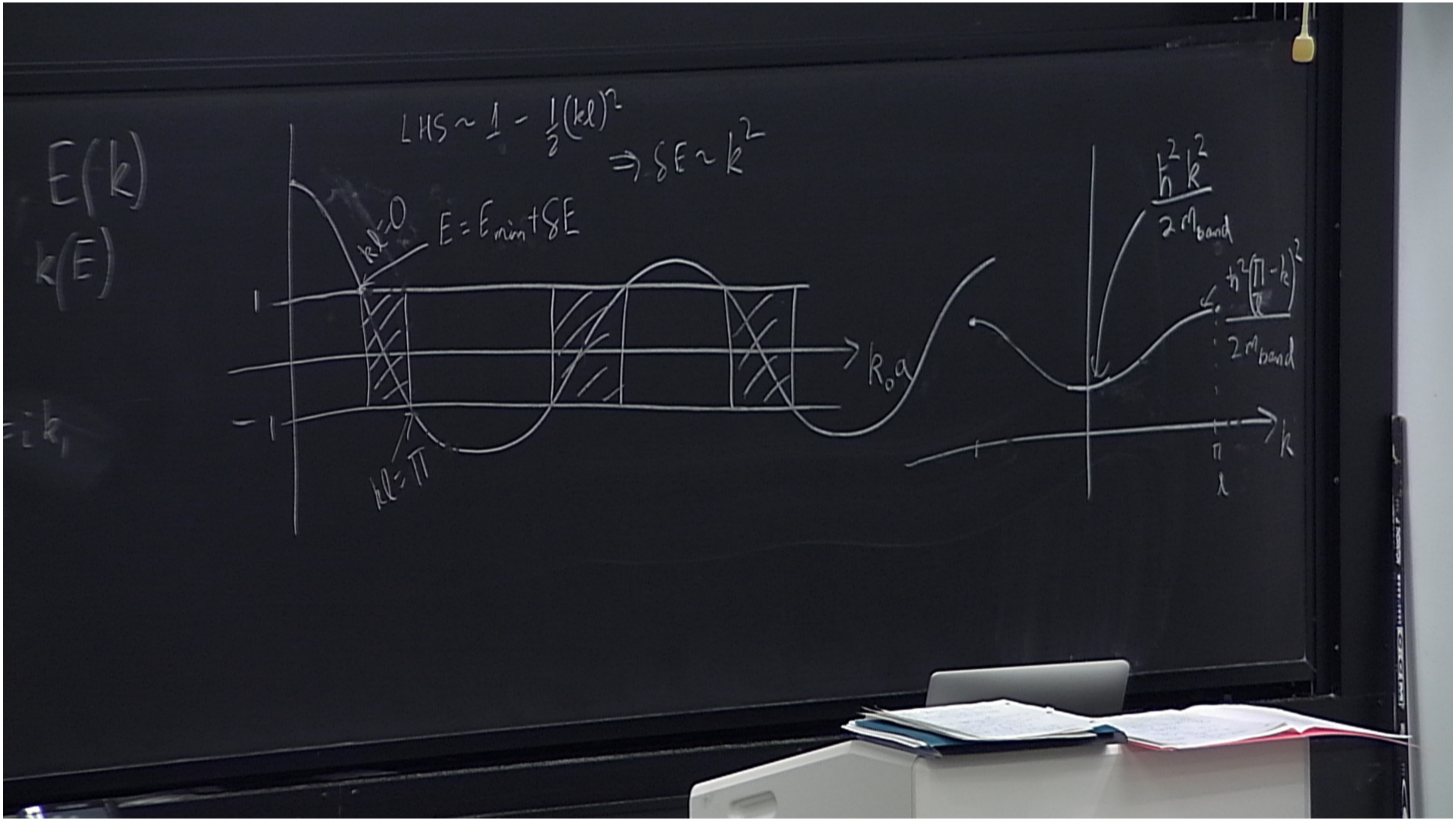

E(k)
k(E)
kℓ=0
1
-1
kℓ=π
$k_0 a$
π/ℓ
k

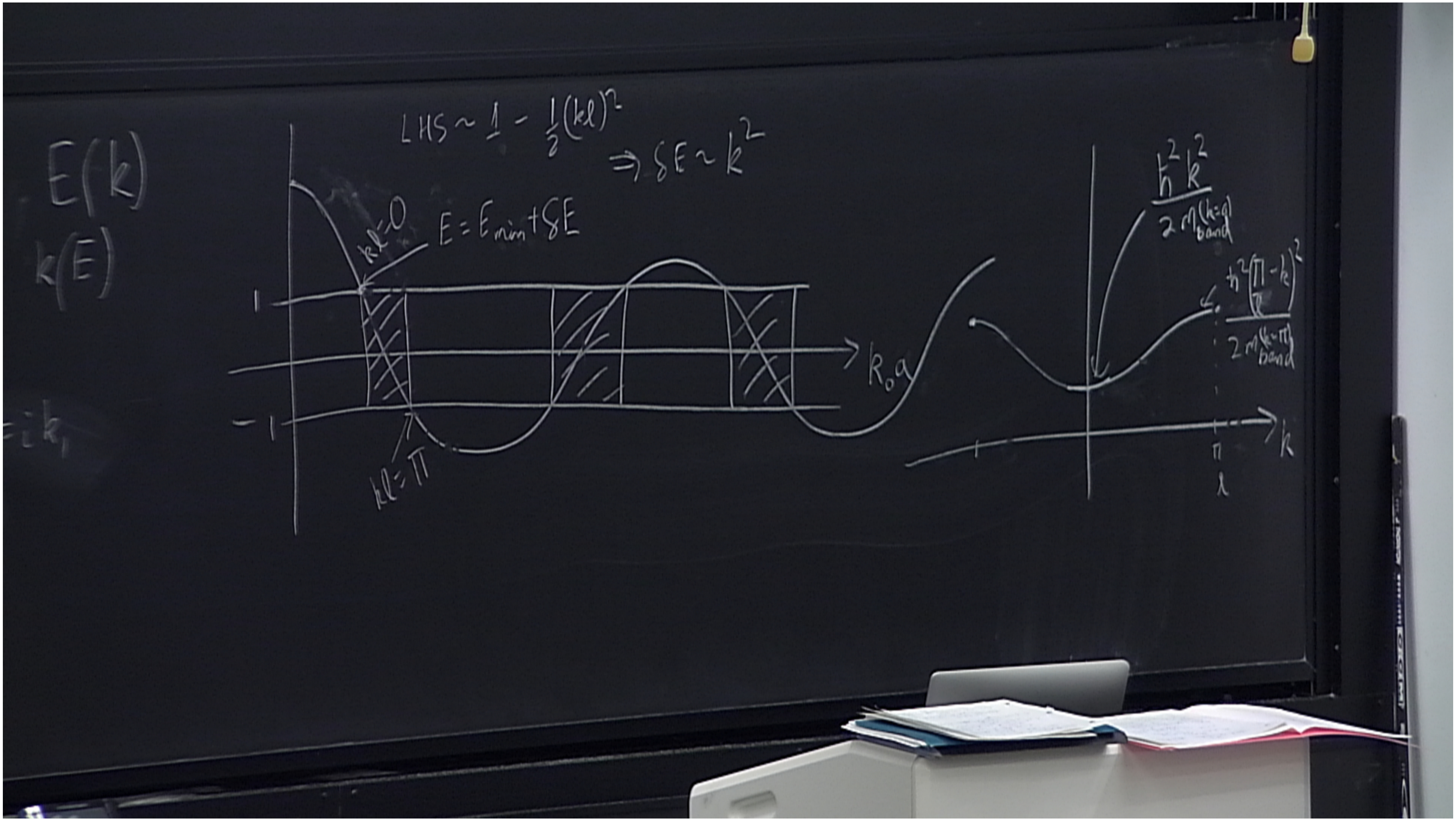

E(k)
k(E)
$kl=0$
$E=E_{min}+\delta E$
1
-1
$k_0 a$
$kl=\pi$


LHS ~ 1 − 1/2 (kl)^2
⇒ δE ~ k^2
E(k)
k(E)
kl = 0
E = E_min + δE
1
−1
k_0 a
kl = π
k
π/l

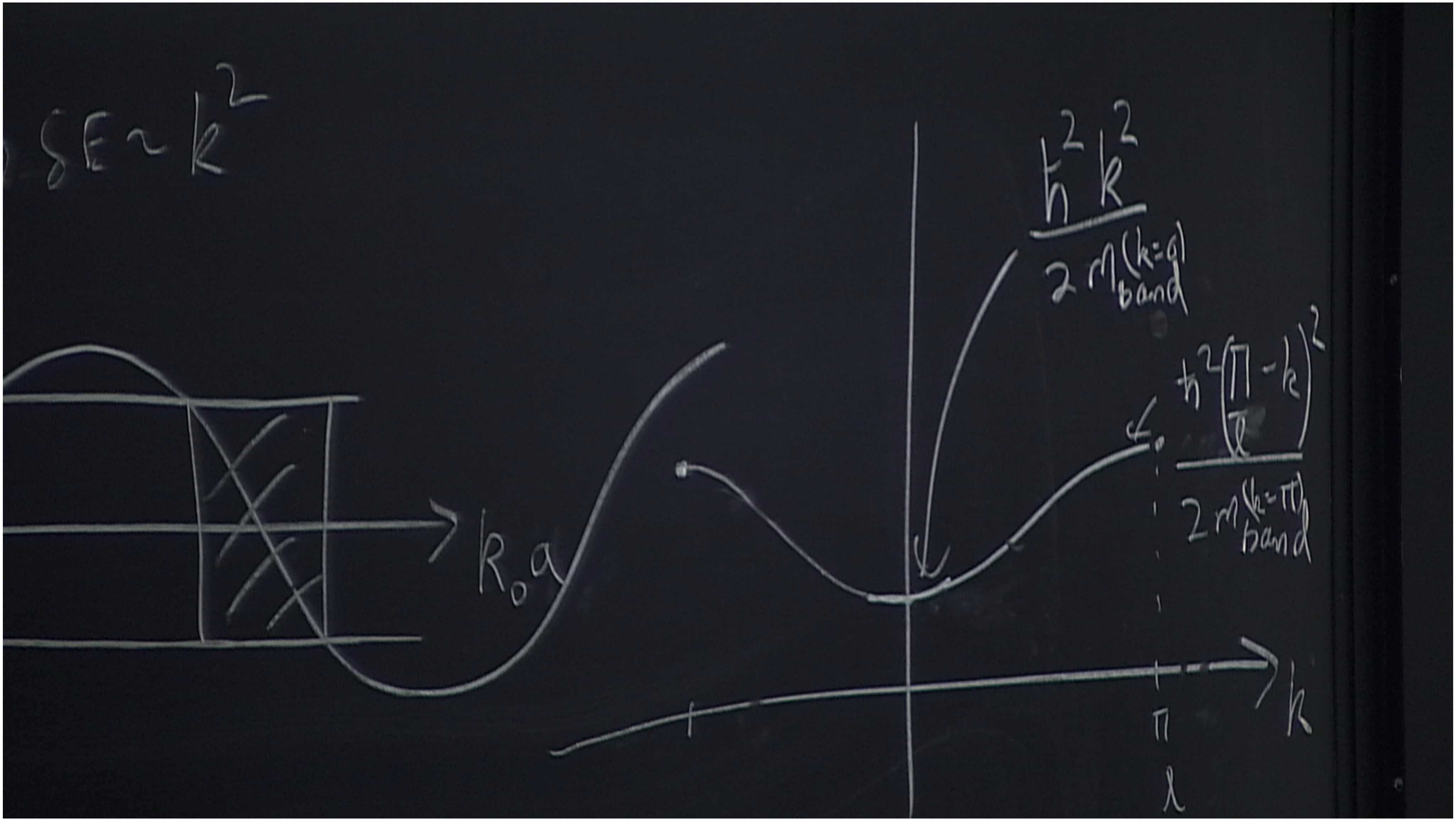


E(k)
k(E)
LHS ~ 1 - 1/2 (kl)^2
⇒ δE ~ k^2
kl=0
E = E_min + δE
kl=π
k_0 a
ħ^2 k^2 / 2m_band
k

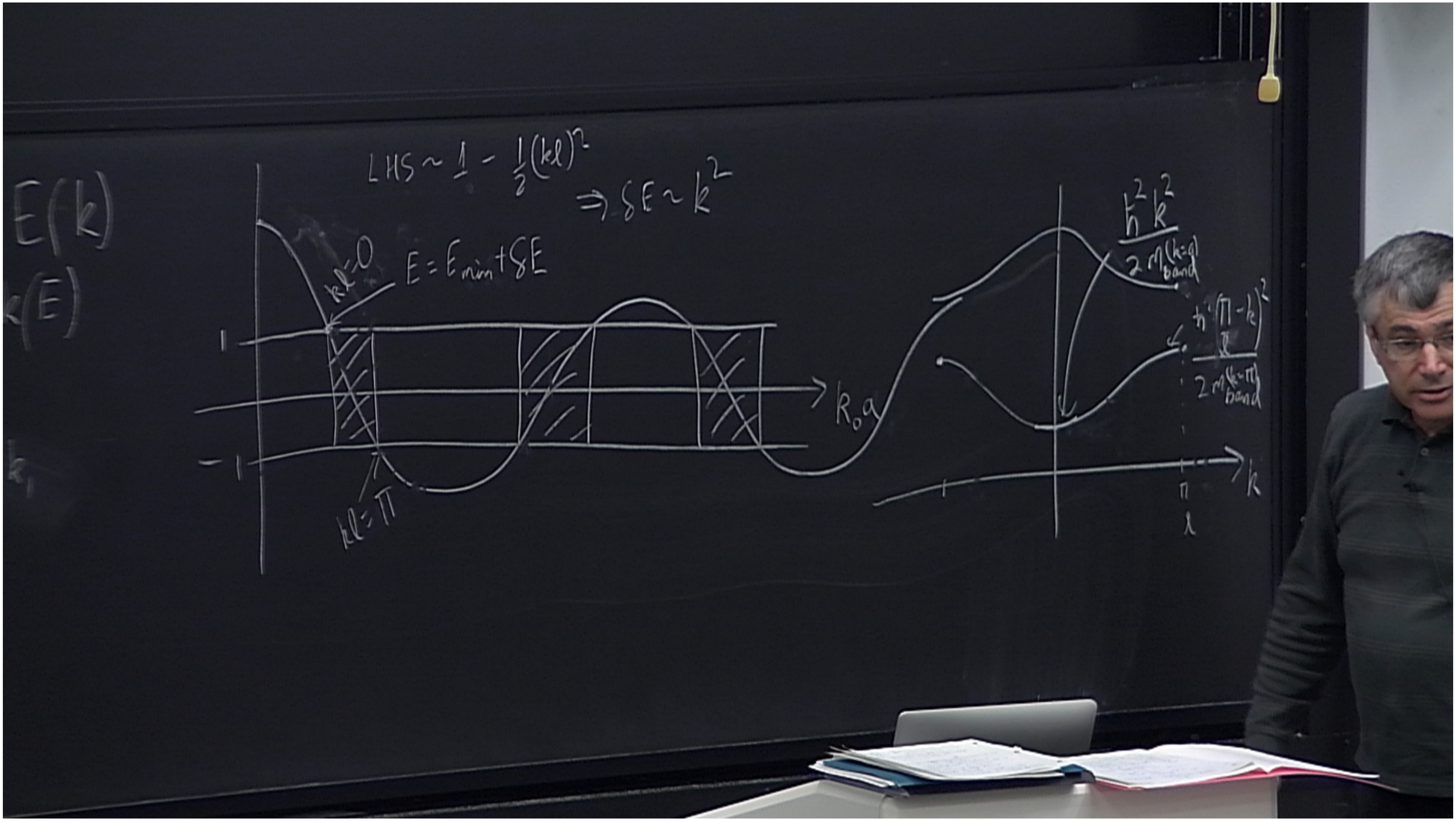

$LHS \sim 1 - \frac{1}{2}(k\ell)^2$
$\Rightarrow \delta E \sim k^2$
$E(k)$
$k(E)$
$k\ell = 0$
$E = E_{min} + \delta E$
$k\ell = \pi$
$R_0 a$
$\frac{\hbar^2 k^2}{2 m_{band}}$
$\frac{\hbar^2(\frac{\pi}{\ell} - k)^2}{2 m_{band}}$
k



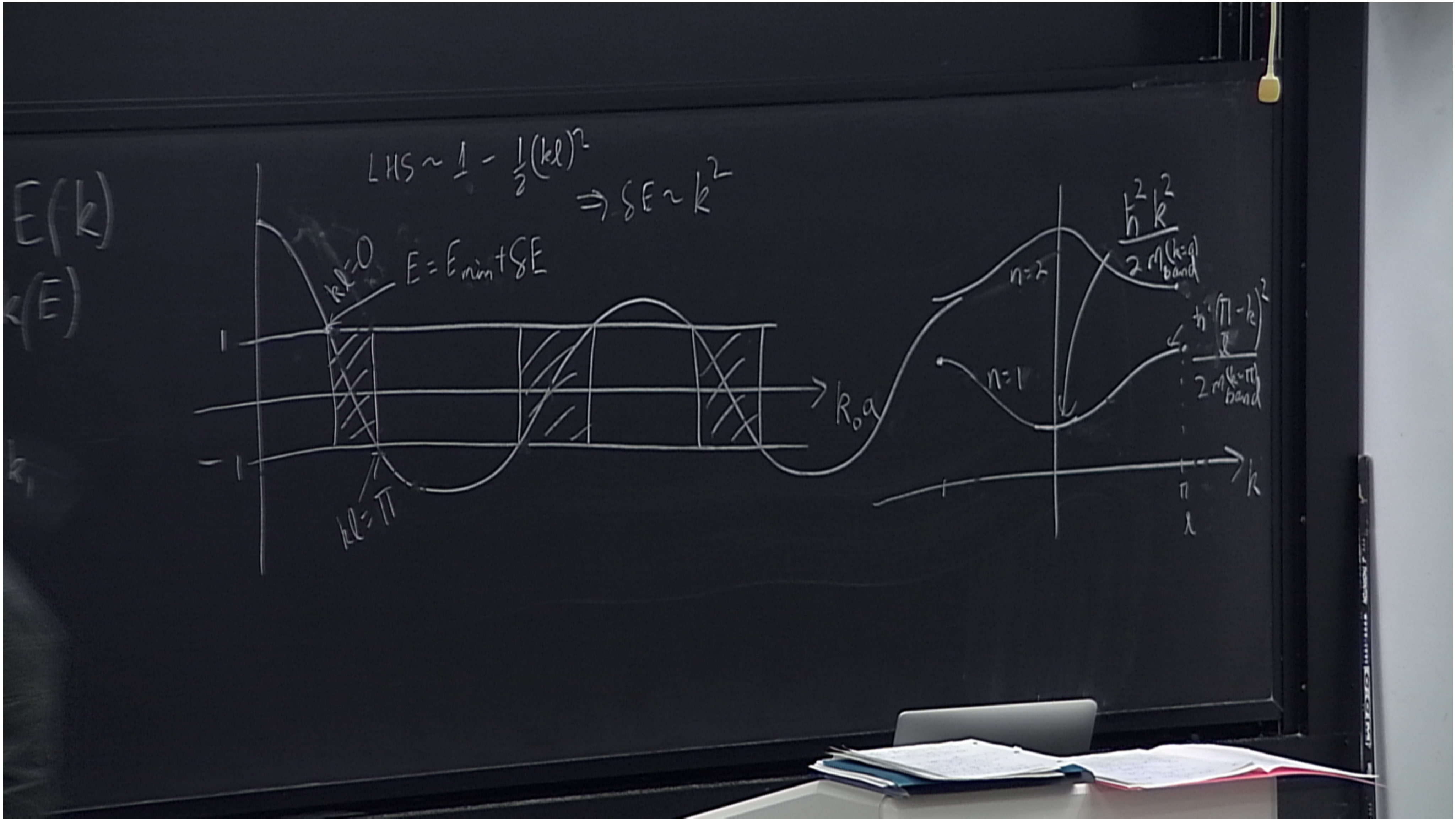
E(k)
k(E)
LHS ~ 1 - ½(kl)²
⇒ δE ~ k²
E = E_min + δE
kl=0
kl=π
k₀a
k



δE ~ k²
R₀a
ħ²k² / 2m_band(k=a)
ħ²(π/ℓ − k)² / 2m_band(k=π/ℓ)
π/ℓ
k



LHS ~ 1 - 1/2 (kℓ)^2
⇒ δE ~ k^2
E(k)
k(E)
E = E_min + δE
kℓ ≈ 0
kℓ = π
1
-1
k_0 a
ħ^2 k^2 / 2 m_band(k=0)
ħ^2 (π - k)^2 / 2 m_band(k=π)
k


LHS ~ 1 - ½(kℓ)²
⇒ δE ~ k²
E(k)
k(E)
kℓ=0
E = E_min + δE
kℓ = π
k₀a
n=2
n=1
ħ²k² / 2m_band(k=0)
ħ²(π/ℓ - k)² / 2m_band(k=π/ℓ)
k

$$\cosh K_1 b \cos k_0 a + \frac{K_1^2 - k_0^2}{2K_1 k_0} \sinh K_1 b \sin k_0 a$$

$E < V_1$

$E(k)$

$k(E)$

$$\underbrace{\cos k_1 b \cos k_0 a - \frac{k_1^2 + k_0^2}{2k_1 k_0} \sin k_1 b \sin k_0 a}_{f(E)}$$

$E > V_1 \quad K_1 = i k_1$

$$k_1 \equiv \sqrt{\frac{2m}{\hbar^2}(E - V_1)}$$

$\sinh k_1 b \sin k_0 a$

$k(E)$

1

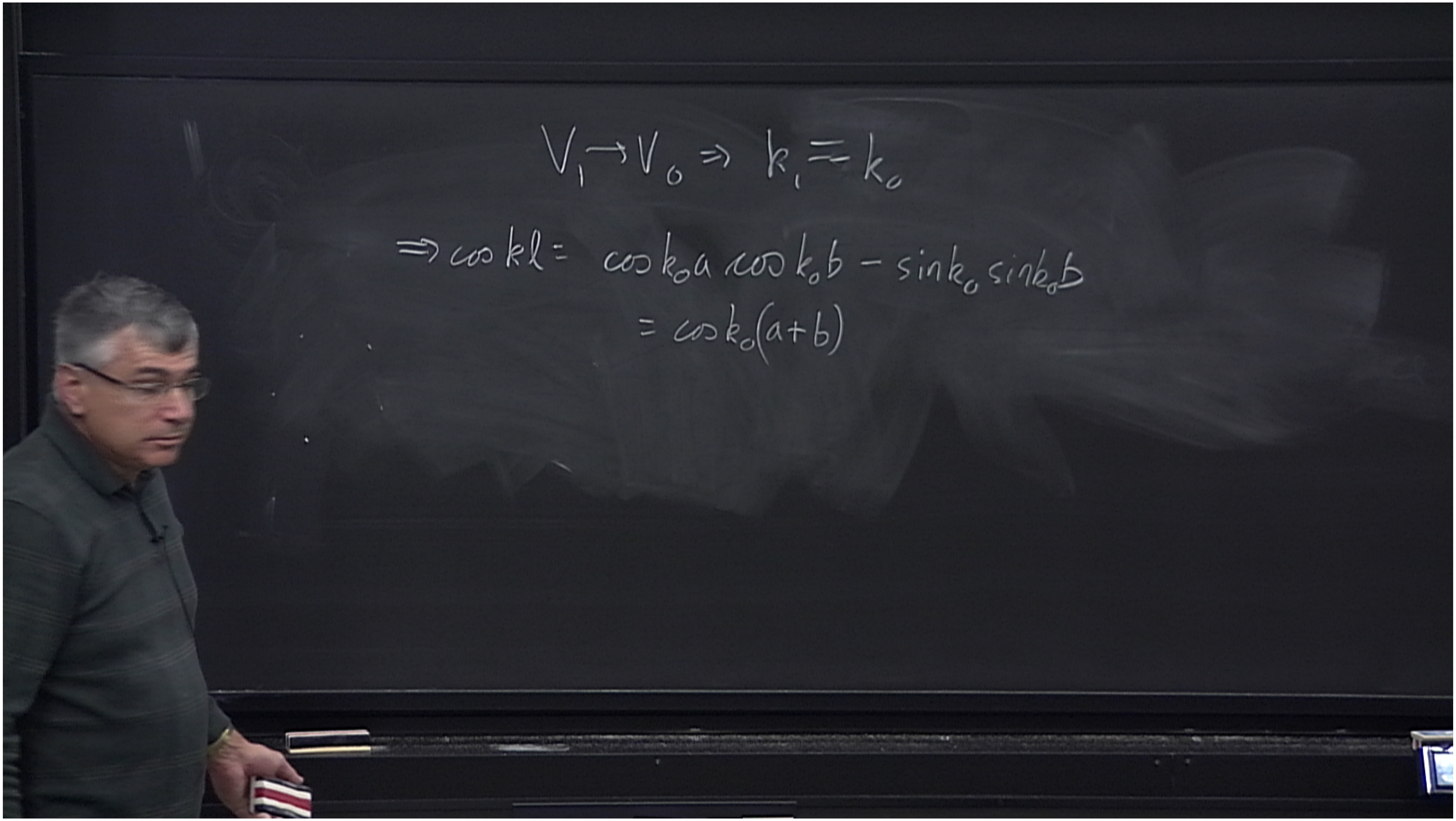
$\sin k_1 b \sin k_0 a$

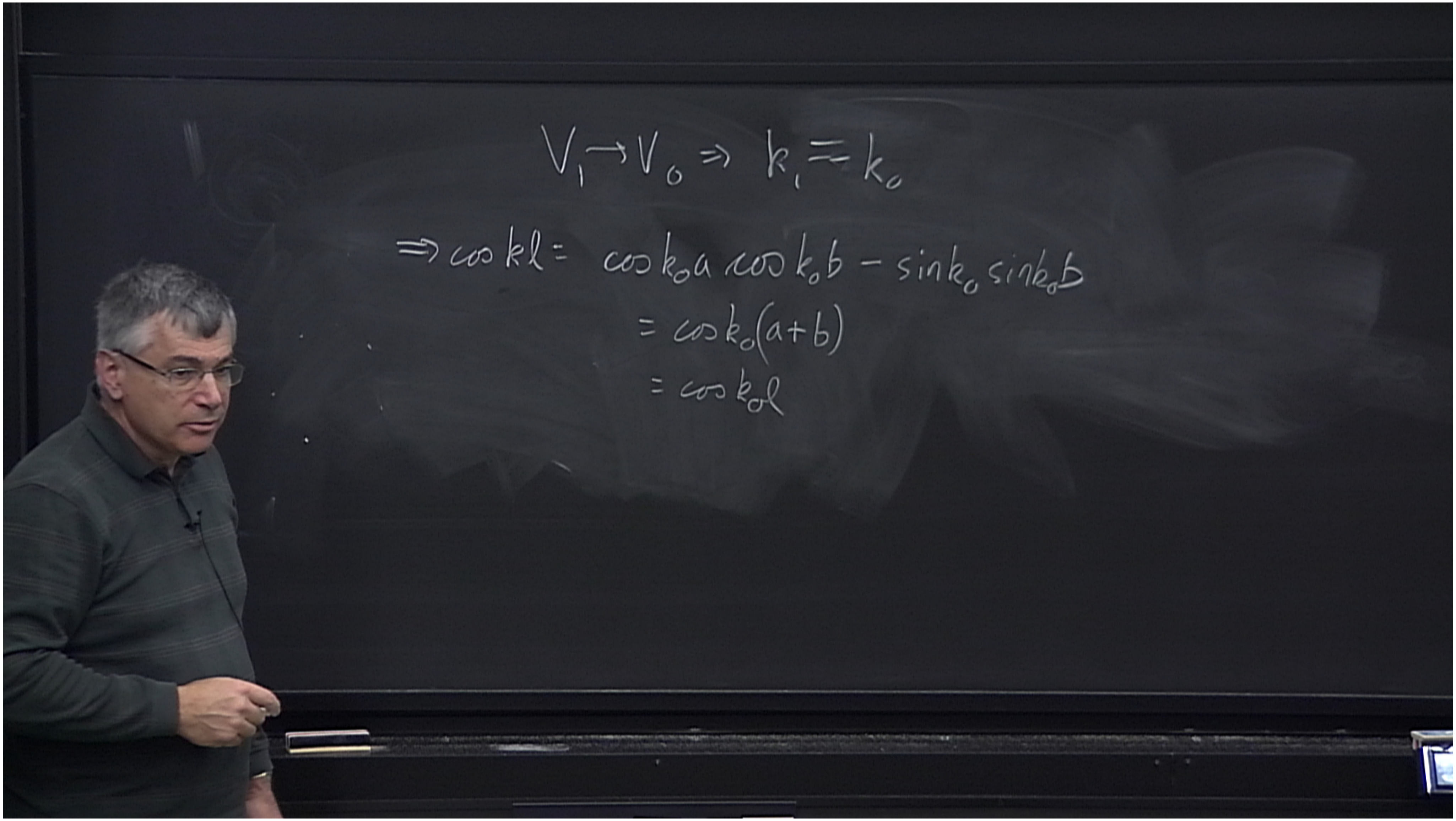
$E > V_1$ $\quad K_1 = i k_1$

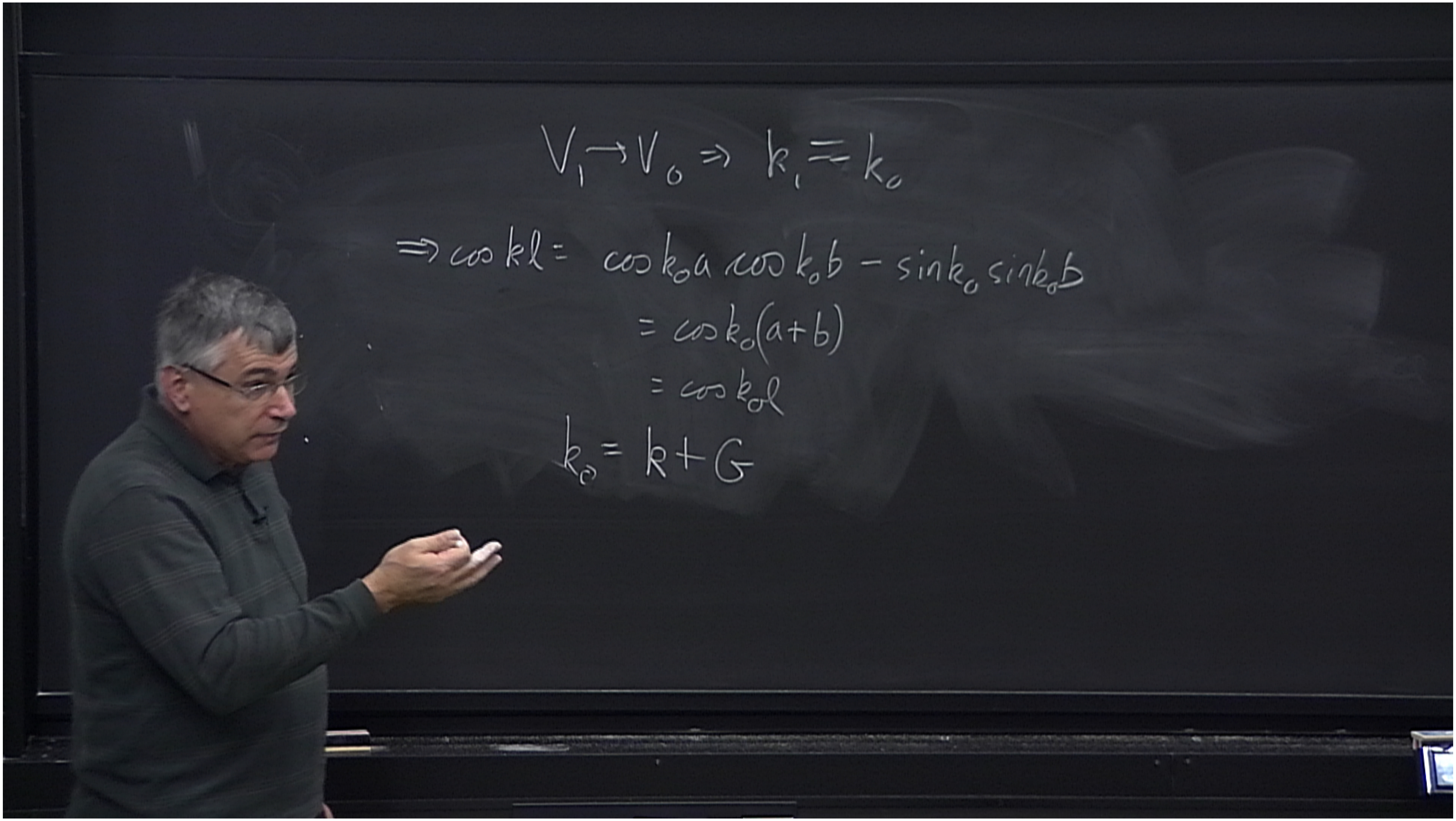
-1

$$k_1 = \sqrt{\frac{2m}{\hbar^2}(E - V_1)}$$

$$V_1 \to V_0 \Rightarrow k_1 = k_0$$


$V_1 \to V_0 \Rightarrow k_1 \to k_0$
$\Rightarrow \cos kl = \cos k_0 a \cos k_0 b - \sin k_0 \sin k_0 b$
$= \cos k_0 (a+b)$


$V_1 \to V_0 \Rightarrow k_1 \to k_0$
$\Rightarrow \cos kl = \cos k_0 a \cos k_0 b - \sin k_0 \sin k_0 b$
$= \cos k_0 (a+b)$
$= \cos k_0 l$


$V_1 \to V_0 \Rightarrow k_1 = k_0$
$\Rightarrow \cos kl = \cos k_0 a \cos k_0 b - \sin k_0 \sin k_0 b$
$= \cos k_0 (a+b)$
$= \cos k_0 l$
$k_0 = k + G$

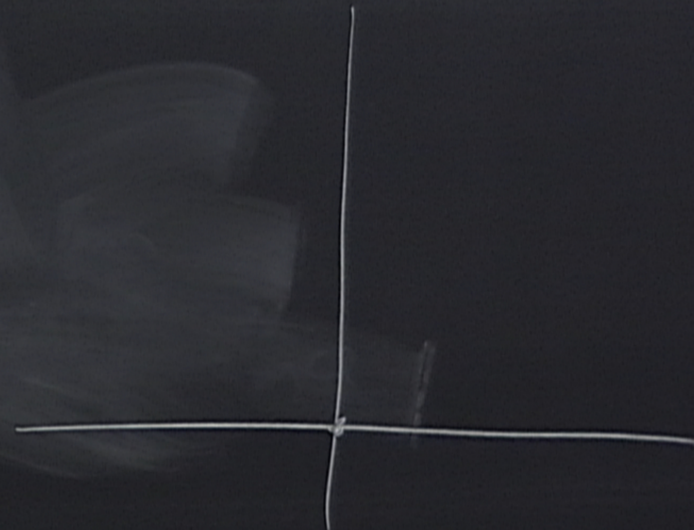
$$V_1 \to V_0 \Rightarrow k_1 \to k_0$$

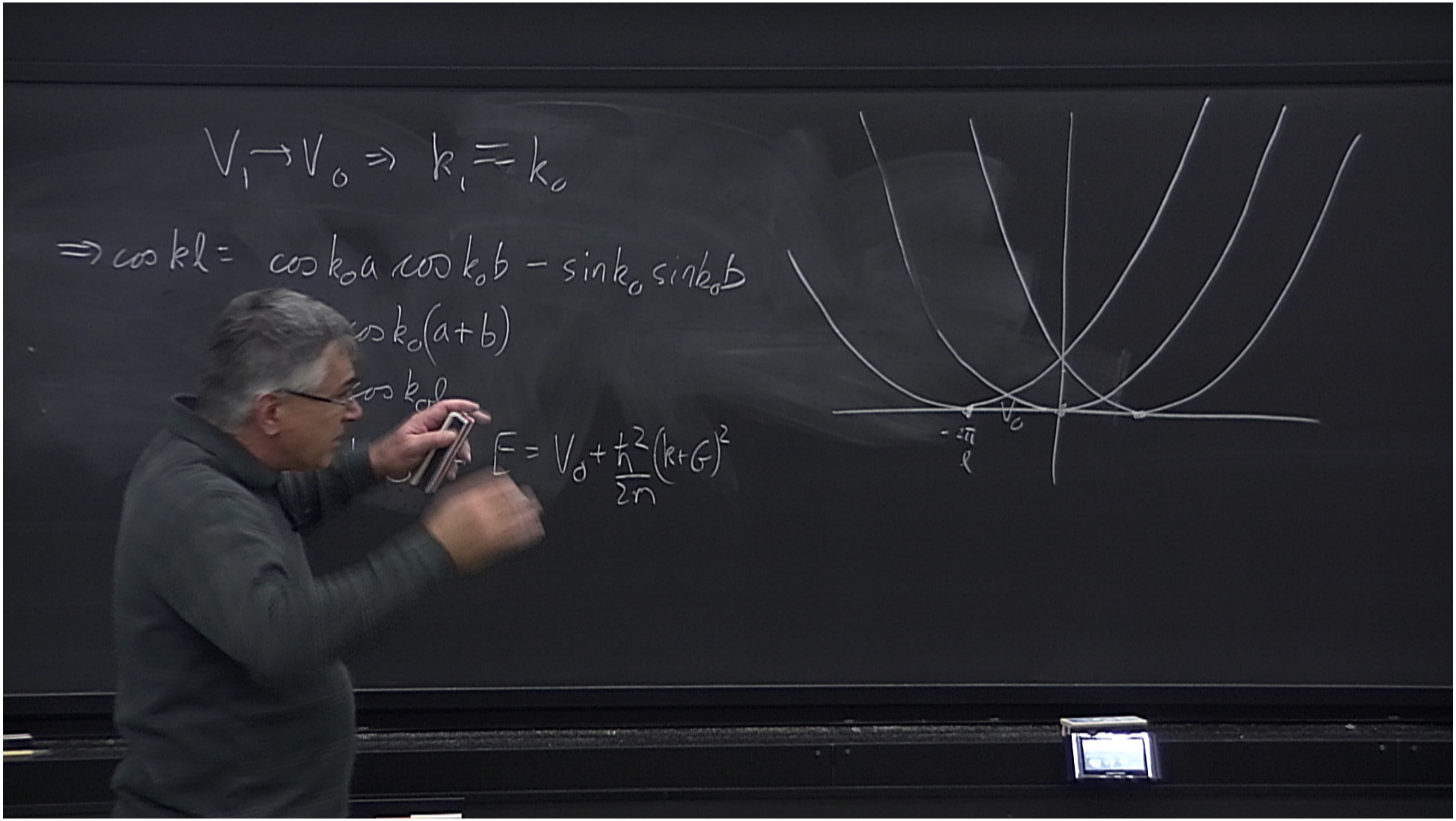
$$\Rightarrow \cos kl = \cos k_0 a \cos k_0 b - \sin k_0 \sin k_0 b$$

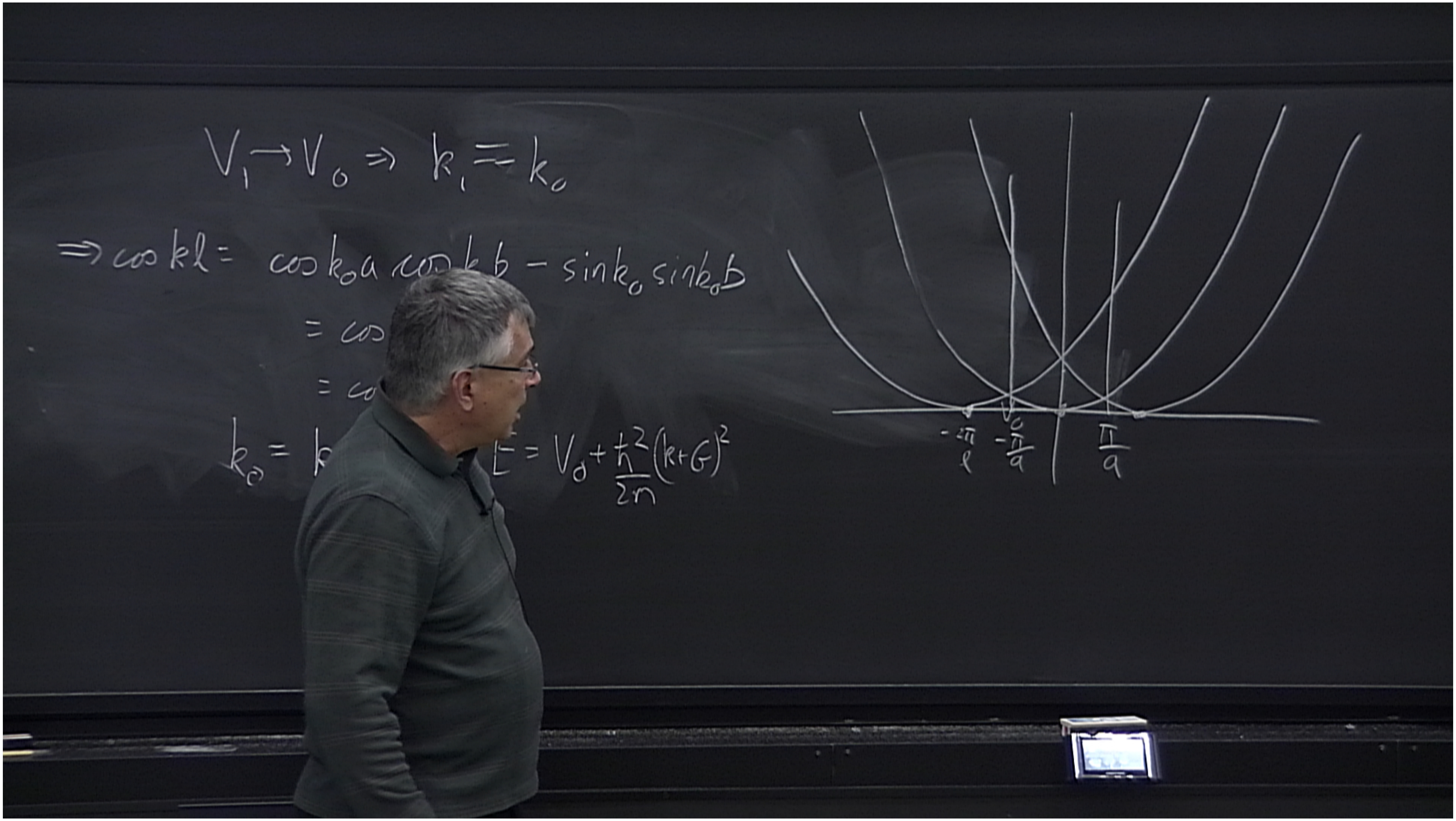
$$= \cos k_0 (a+b)$$

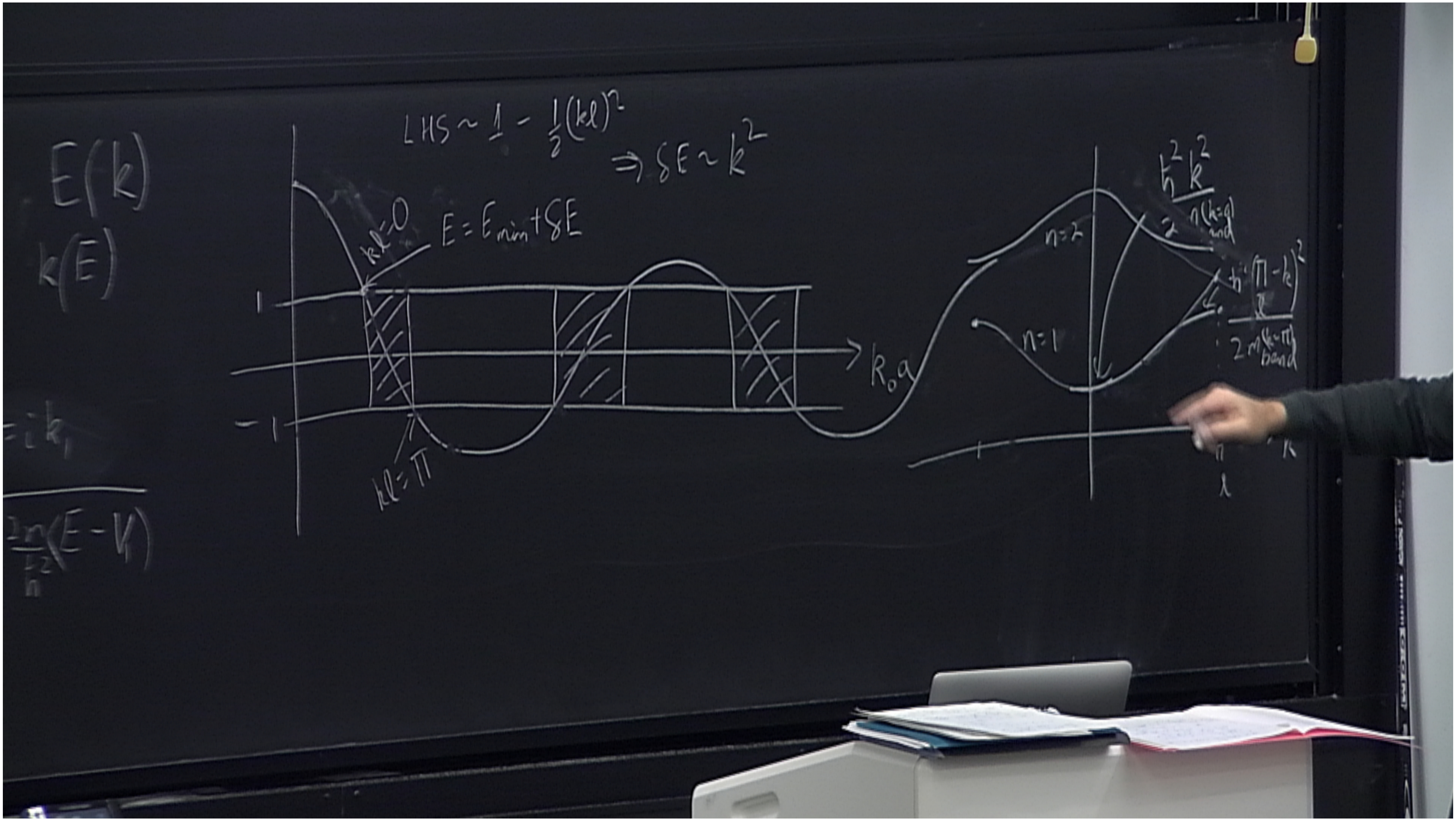
$$= \cos k_0 l$$

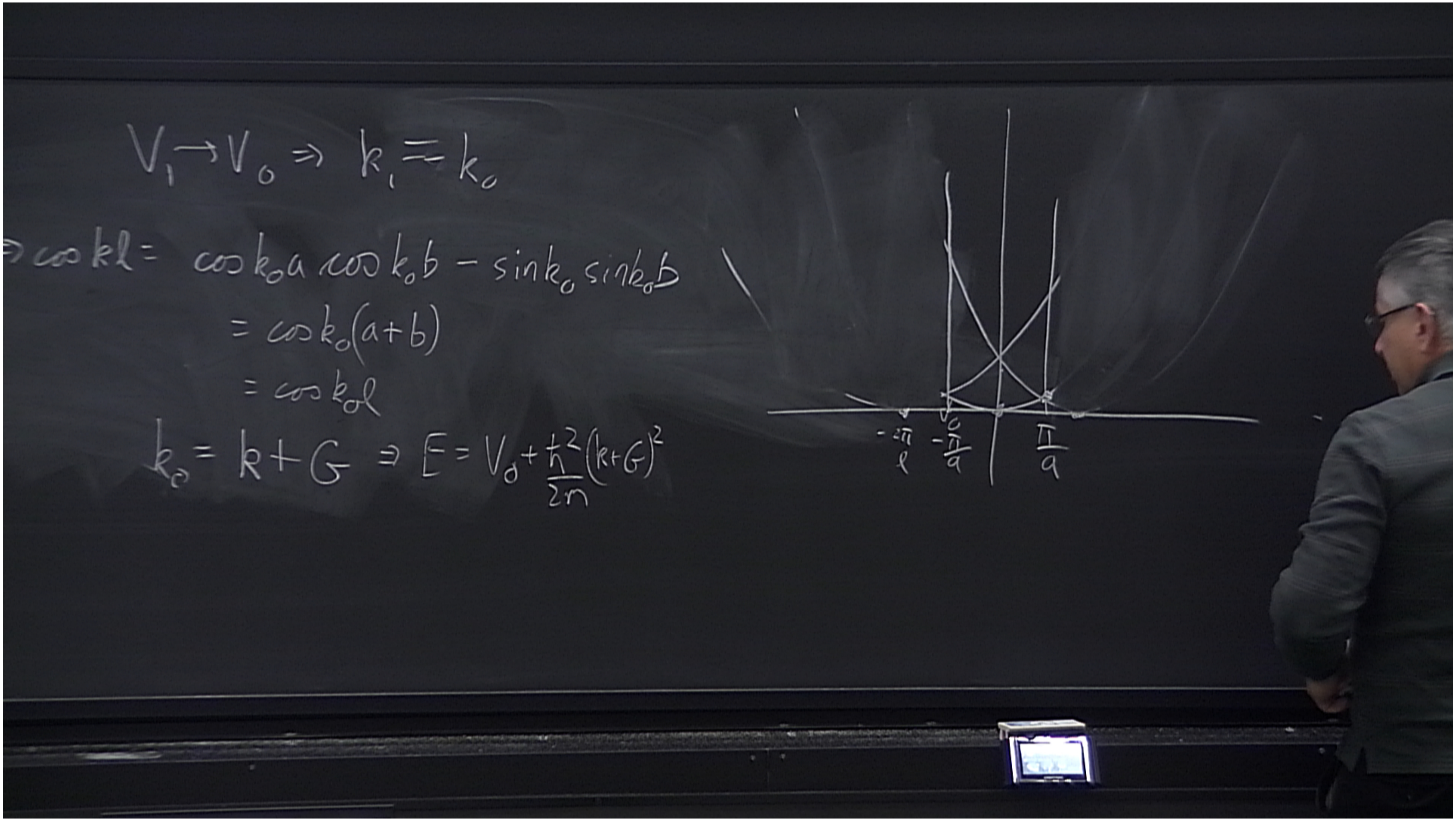
$$k_0 = k + G \Rightarrow E = V_0 + \frac{\hbar^2}{2m}(k+G)^2$$



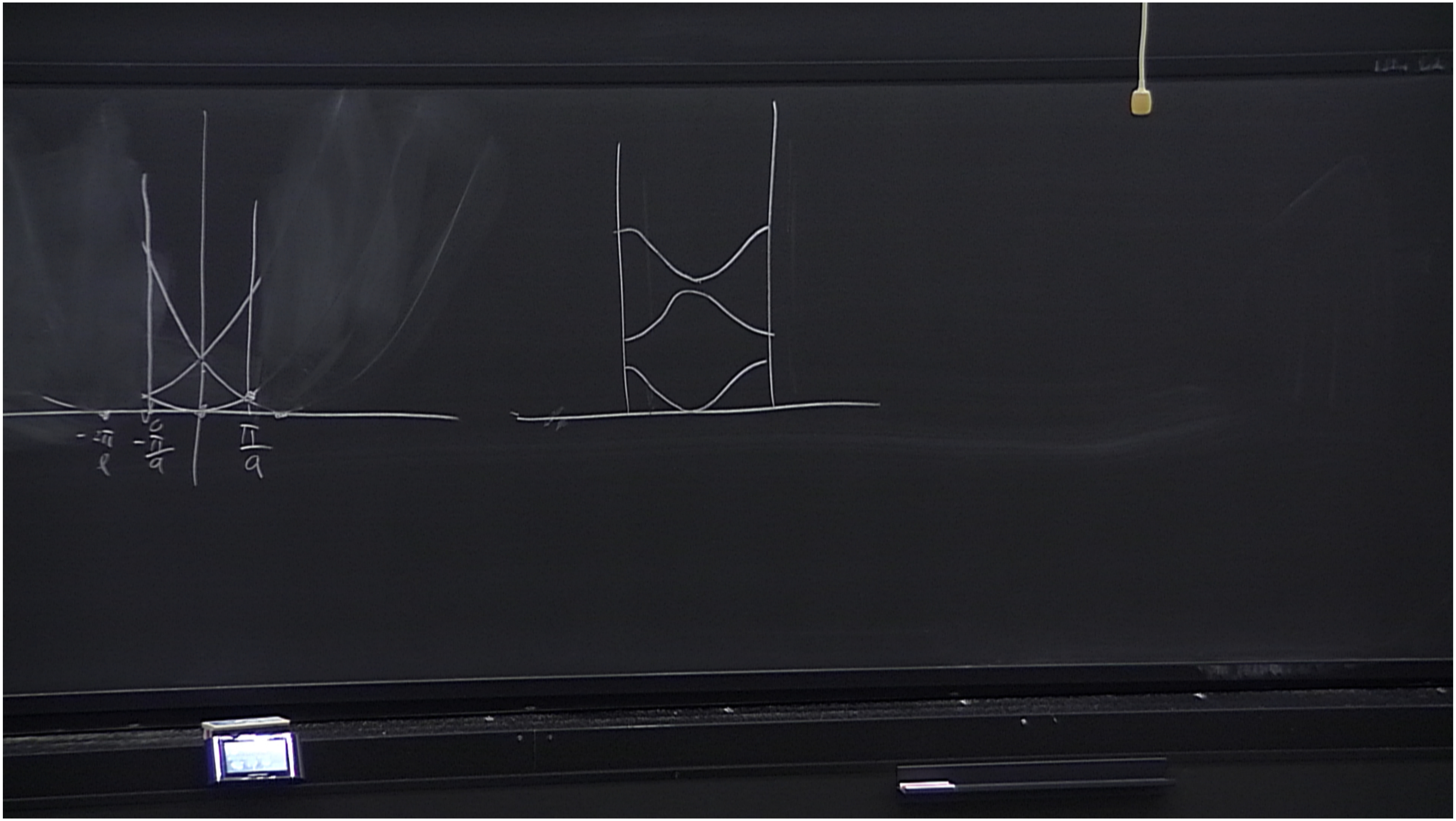

$V_1 \to V_0 \Rightarrow k_1 = k_0$
$\Rightarrow \cos kl = \cos k_0 a \cos k_0 b - \sin k_0 \sin k_0 b$
$\cos k_0(a+b)$
$\cos k_0 l$
$E = V_0 + \frac{\hbar^2}{2m}(k+G)^2$
V_0
$-\frac{2\pi}{l}$

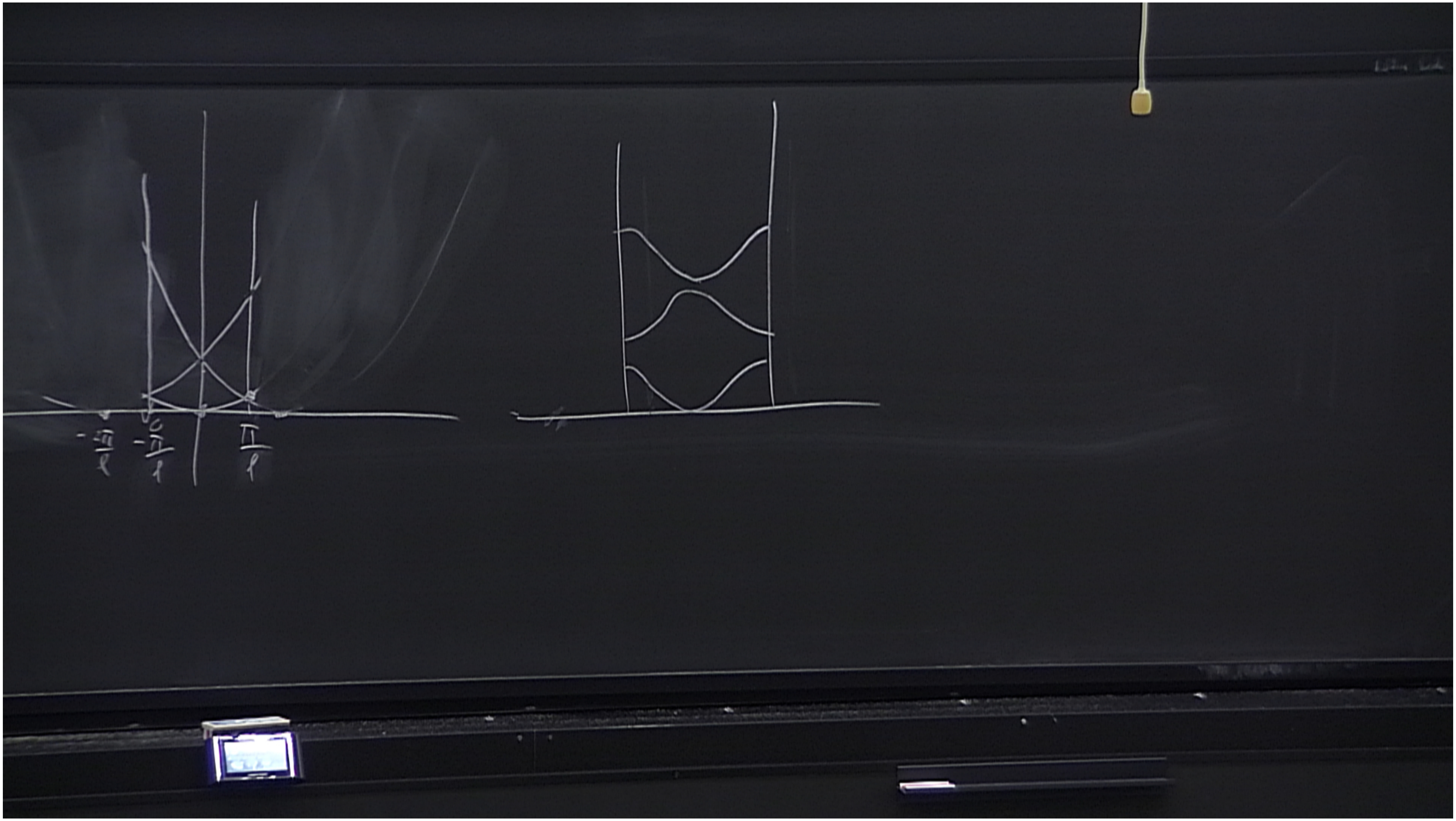

$V_1 \to V_0 \Rightarrow k_1 = k_0$
$\Rightarrow \cos kl = \cos k_0 a \cos k_0 b - \sin k_0 \sin k_0 b$
$E = V_0 + \frac{\hbar^2}{2m}(k+G)^2$
V_0
$-\frac{2\pi}{l}$
$-\frac{\pi}{a}$
$\frac{\pi}{a}$

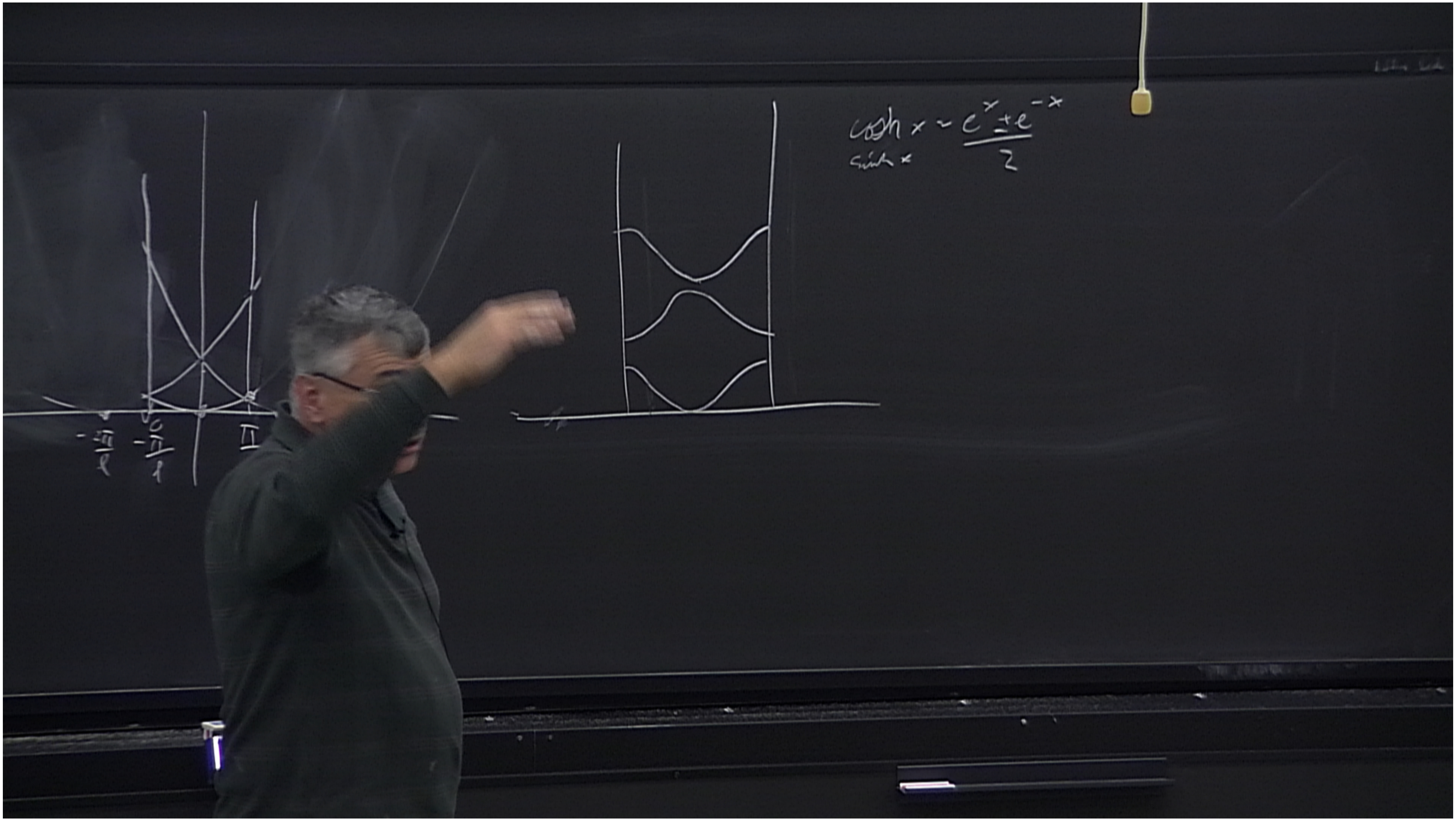

E(k)
k(E)
LHS ~ 1 - ½(kℓ)²
⇒ δE ~ k²
kℓ=0
E = E_min + δE
kℓ = π
R₀a
n=2
n=1

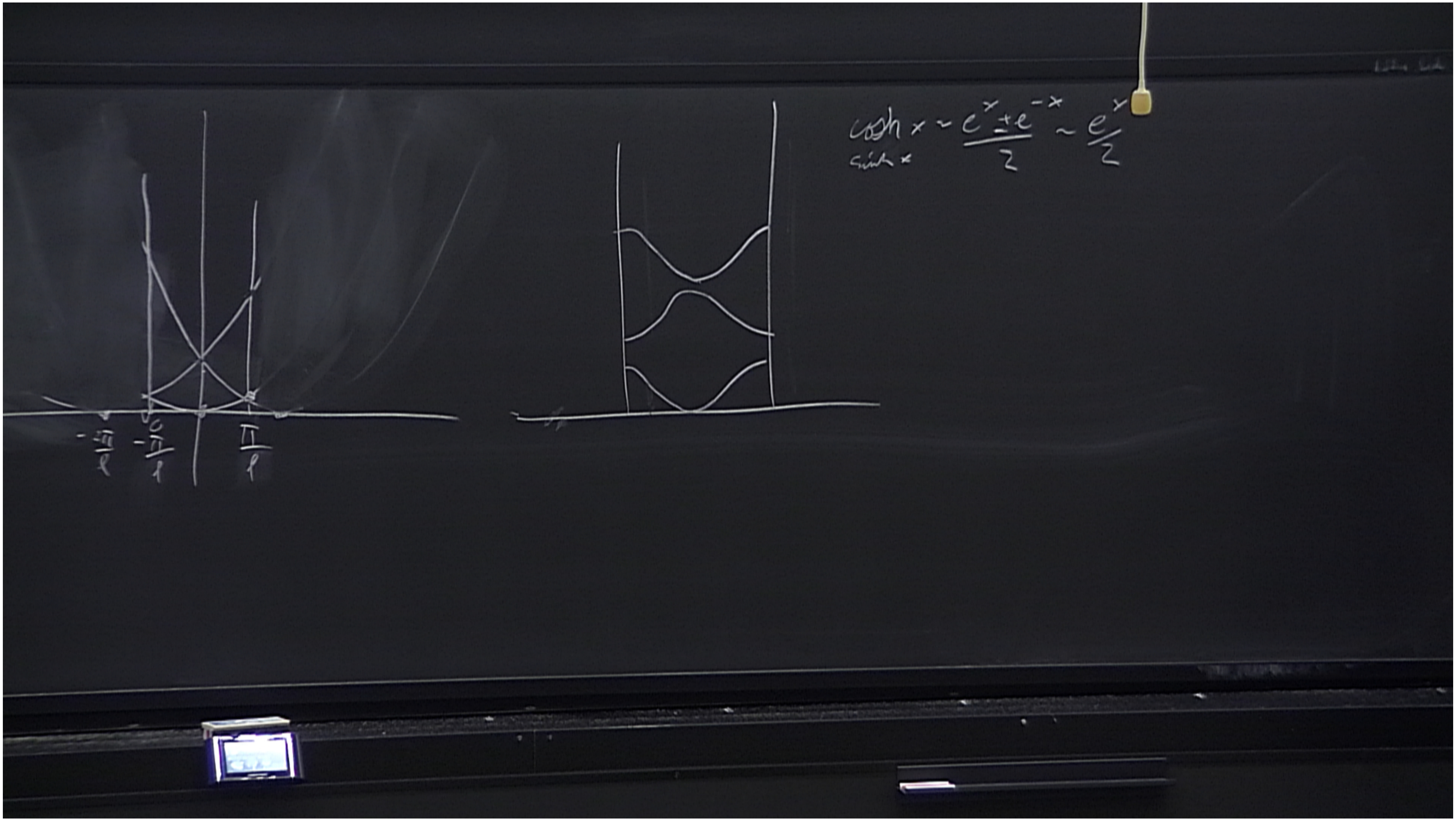


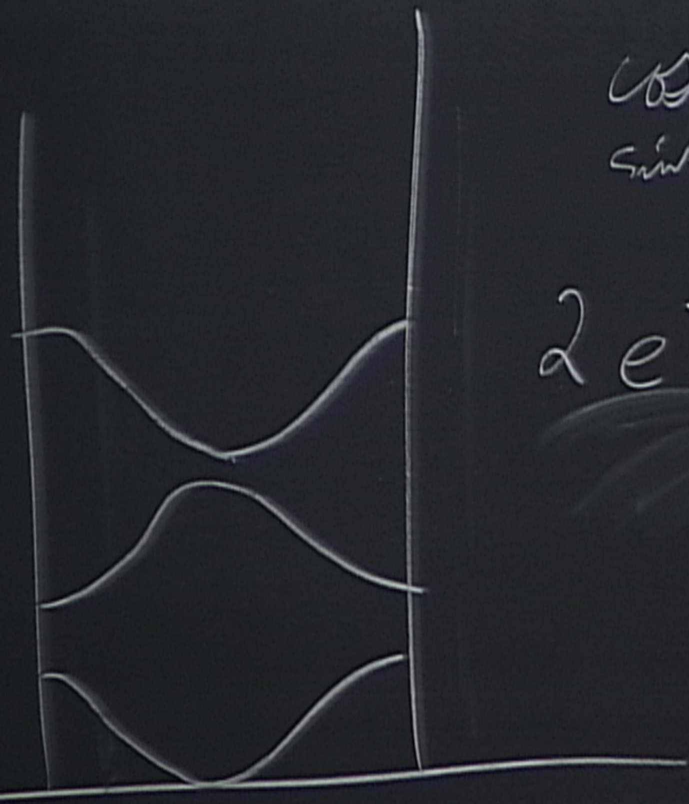
$V_1 \to V_0 \Rightarrow k_1 = k_0$
$\Rightarrow \cos kl = \cos k_0 a \cos k_0 b - \sin k_0 \sin k_0 b$
$= \cos k_0 (a+b)$
$= \cos k_0 l$
$k_0 = k + G \Rightarrow E = V_0 + \frac{\hbar^2}{2m}(k+G)^2$
V_0
$-\frac{2\pi}{l}$
$-\frac{\pi}{a}$
$\frac{\pi}{a}$


$-\frac{\pi}{\ell}$
$-\frac{\pi}{a}$
$\frac{\pi}{a}$


$-\frac{\pi}{\ell}$
$\frac{\pi}{\ell}$


cosh x = (e^x ± e^-x)/2
sinh x

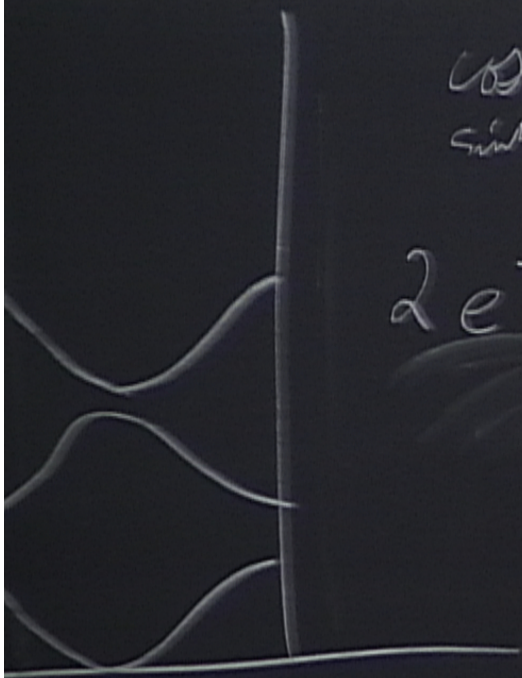

cosh x ~ e^x ± e^-x / 2 ~ e^x / 2
sinh x
-π/ℓ
-π/ℓ
π/ℓ



$$\cosh x \sim \frac{e^{x} \pm e^{-x}}{2} \sim \frac{e^{x}}{2}$$

$\sinh x$

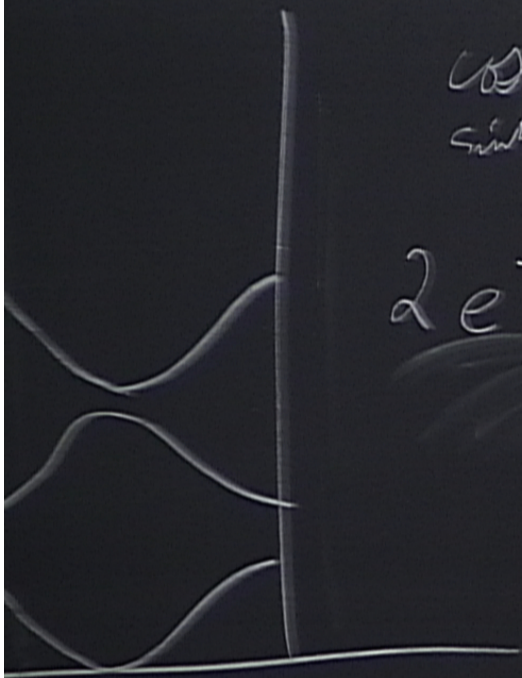
$$2e^{-\kappa_1 b}\cos kl \approx \cos k_0 a$$



$$\cosh x \sim \frac{e^{x} \pm e^{-x}}{2} \sim \frac{e^{x}}{2}$$

$\sinh x$

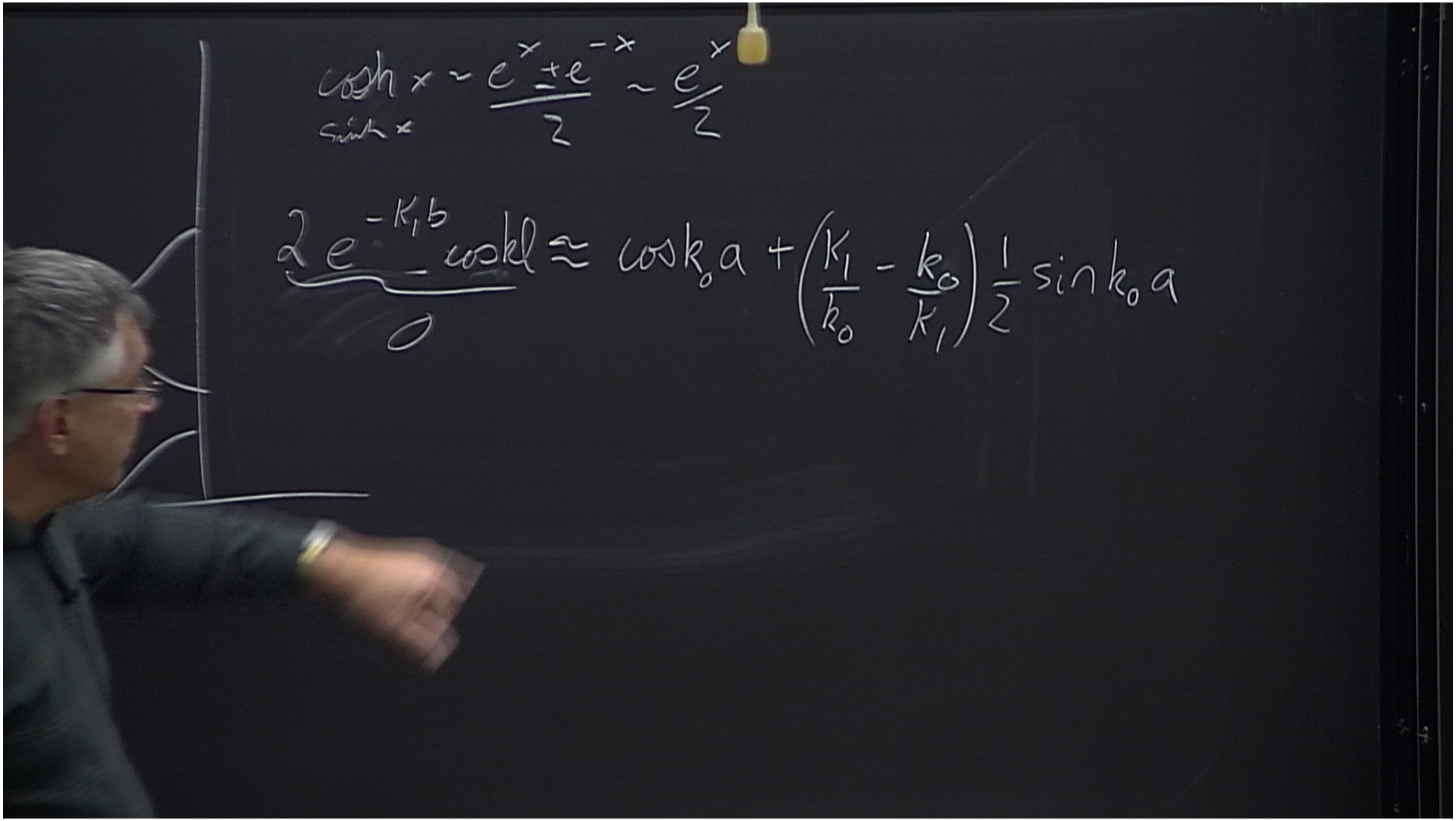
$$2 e^{-\kappa_1 b} \cos kl \simeq \cos k_0 a + \left(\frac{\kappa_1}{k_0} - \frac{k_1}{\kappa_1}\right)\frac{1}{2} \sin k_0 a$$



$$\cosh x \sim \frac{e^{x} + e^{-x}}{2} \sim \frac{e^{x}}{2}$$

$\sinh x$

$$2 e^{-K_1 b} \cos kl \approx \cos k_0 a + \left(\frac{K_1}{k_0} - \frac{k_0}{K_1}\right)\frac{1}{2} \sin k_0 a$$


$\cosh x \sim \frac{e^{x}+e^{-x}}{2} \sim \frac{e^{x}}{2}$
$\sinh x$
$2e^{-K_1 b}\cos kl \approx \cos k_0 a + \left(\frac{K_1}{k_0} - \frac{k_0}{K_1}\right)\frac{1}{2}\sin k_0 a$
0

$$\cosh x \sim \frac{e^{x} + e^{-x}}{2} \sim \frac{e^{x}}{2}$$

$\sinh x$

$$\underbrace{2e^{-K_1 b}\cos kl}_{0} \approx \cos k_0 a + \left(\frac{K_1}{k_0} - \frac{k_0}{K_1}\right)\frac{1}{2}\sin k_0 a$$

$$\cos^2 \frac{k_0 a}{2} - \sin^2 \frac{k_0 a}{2}$$

$$\cosh x \sim \frac{e^{x} + e^{-x}}{2} \sim \frac{e^{x}}{2}$$

$\sinh x$

$$\underbrace{2 e^{-K_1 b} \cos kl}_{0} \approx \cos k_0 a + \left(\frac{K_1}{k_0} - \frac{k_0}{K_1}\right)\frac{1}{2}\sin k_0 a$$

$$\cos^2 \frac{k_0 a}{2} - \sin^2 \frac{k_0 a}{2} + \left(\frac{K_1}{k_0} - \frac{k_0}{K_1}\right) \sin \frac{k_0 a}{2} \cos \frac{k_0 a}{2}$$

$$\cosh x \sim \frac{e^{x} + e^{-x}}{2} \sim \frac{e^{x}}{2}$$

$\sinh x$

$$\underbrace{2 e^{-K_1 b}}_{0} \cos kl \approx \cos k_0 a + \left(\frac{K_1}{k_0} - \frac{k_0}{K_1}\right)\frac{1}{2} \sin k_0 a$$

$$\cos^2 \frac{k_0 a}{2} - \sin^2 \frac{k_0 a}{2} + \left(\frac{K_1}{k_0} - \frac{k_0}{K_1}\right) \sin \frac{k_0 a}{2} \cos \frac{k_0 a}{2}$$

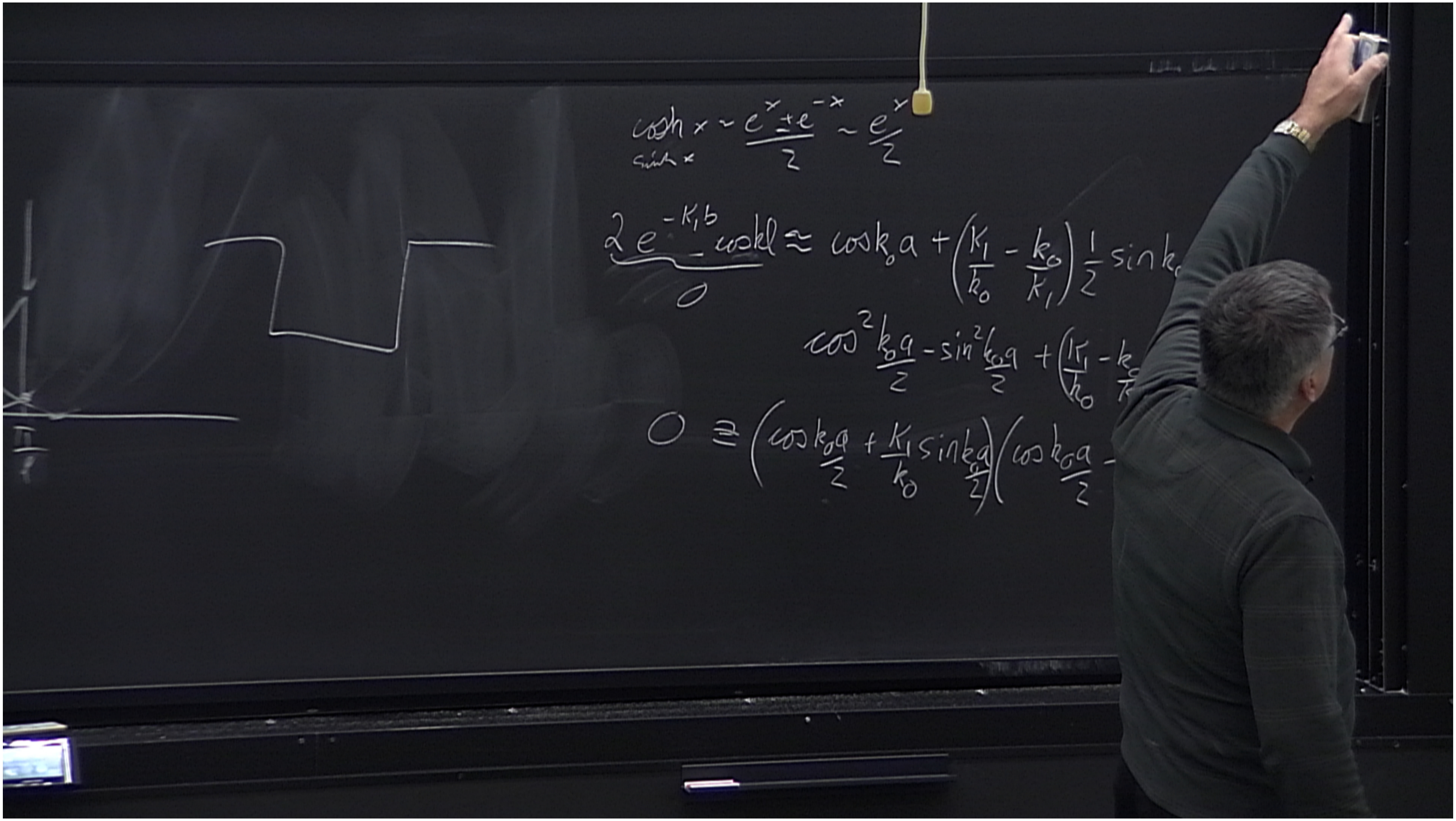
$$\left(\cos \frac{k_0 a}{2} + \frac{K_1}{k_0} \sin \frac{k_0 a}{2}\right)\left(\cos \frac{k_0 a}{2} - \frac{k_0}{K_1} \sin \frac{k_0 a}{2}\right)$$

$$\begin{matrix}\cosh x \\ \sinh x\end{matrix} \sim \frac{e^{x} \pm e^{-x}}{2} \sim \frac{e^{x}}{2}$$

$$\underbrace{2e^{-\kappa_1 b}}_{0} \cos kl \approx \cos k_0 a + \left(\frac{\kappa_1}{k_0} - \frac{k_0}{\kappa_1}\right)\frac{1}{2}\sin k_0 a$$

$$\cos^2\frac{k_0 a}{2} - \sin^2\frac{k_0 a}{2} + \left(\frac{\kappa_1}{k_0} - \frac{k_0}{\kappa_1}\right)\sin\frac{k_0 a}{2}\cos\frac{k_0 a}{2}$$

$$\left(\cos\frac{k_0 a}{2} + \frac{\kappa_1}{k_0}\sin\frac{k_0 a}{2}\right)\left(\cos\frac{k_0 a}{2} - \frac{k_0}{\kappa_1}\sin\frac{k_0 a}{2}\right)$$



cosh x ~ (e^x ± e^-x)/2 ~ e^x/2
sinh x
2e^(-K_1 b) cos kl ≈ cos k_0 a + (K_1/k_0 - k_0/K_1) 1/2 sin k
0
cos^2 (k_0 a/2) - sin^2 (k_0 a/2) + (K_1/k_0 - k
0 ≅ (cos (k_0 a/2) + (K_1/k_0) sin (k_0 a/2))(cos (k_0 a/2) -