Title: PSI 2015/2016 Condensed Matter - Oleg Tchernyshyov - Lecture 5

Date: Nov 13, 2015 10:45 AM

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Abstract:

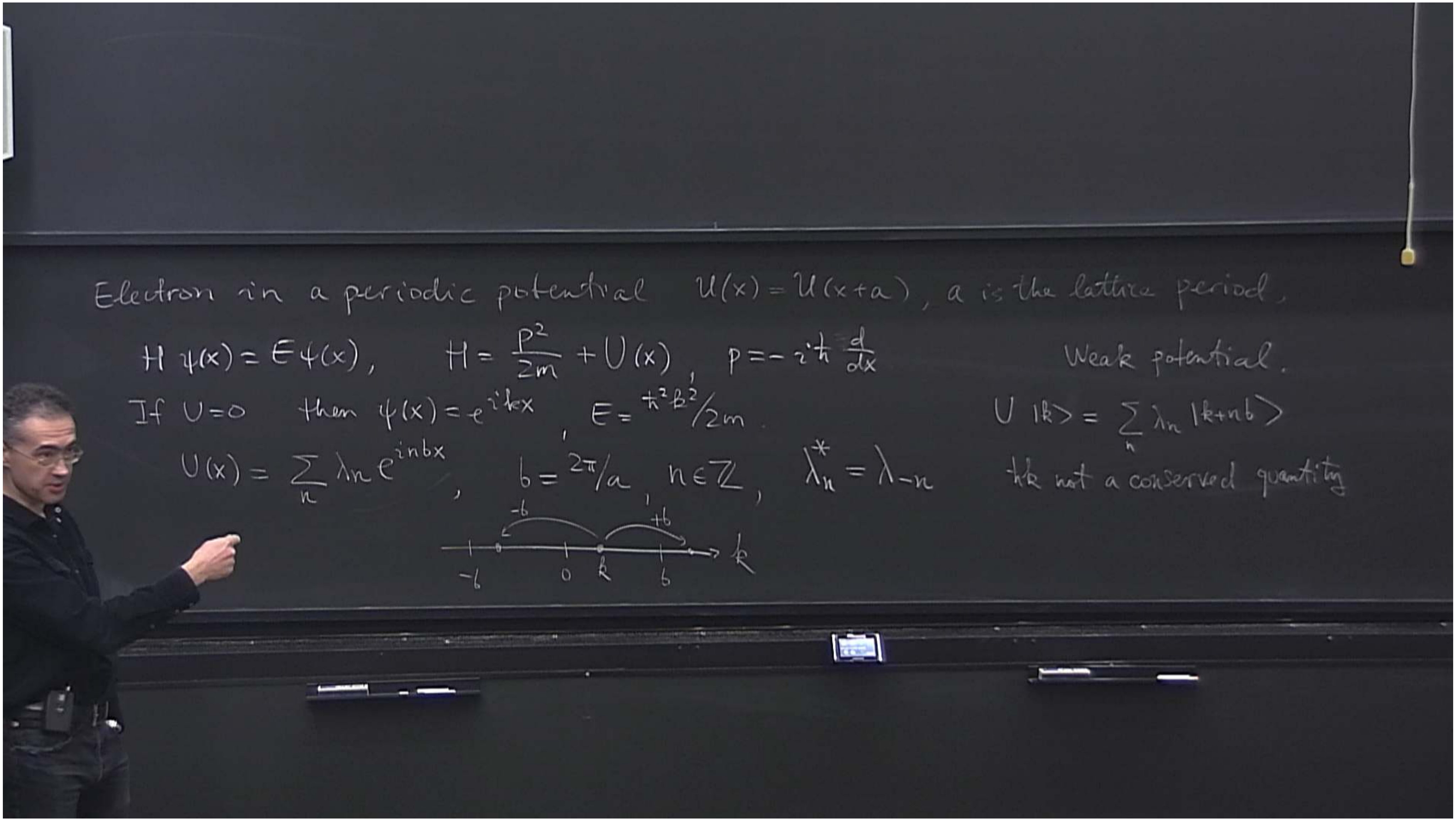
Electrons in a periodic lattice

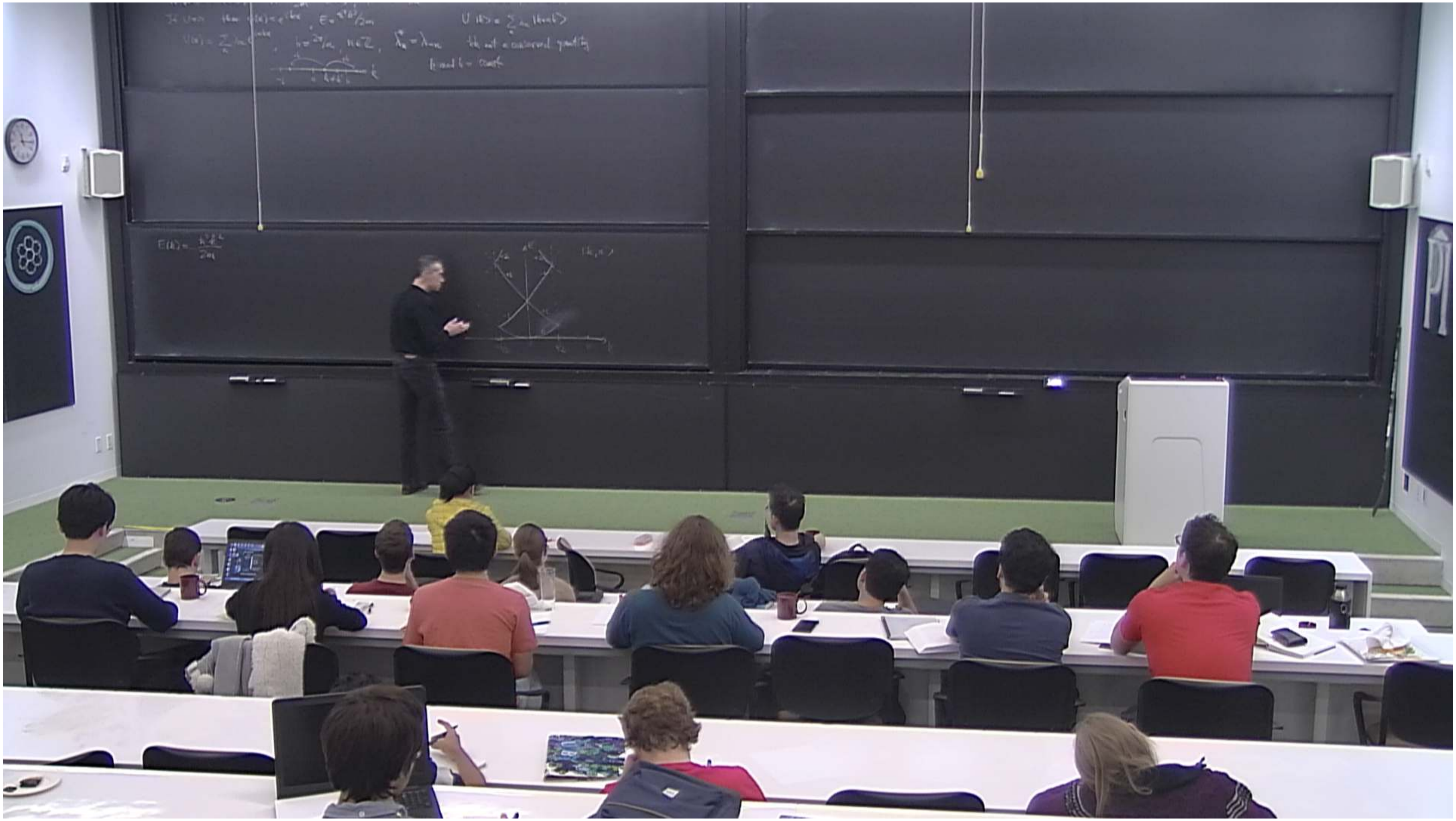
1. One spatial dimension.
2. Energy gaps.
3. Higher dimensions.
4. Reciprocal lattice.

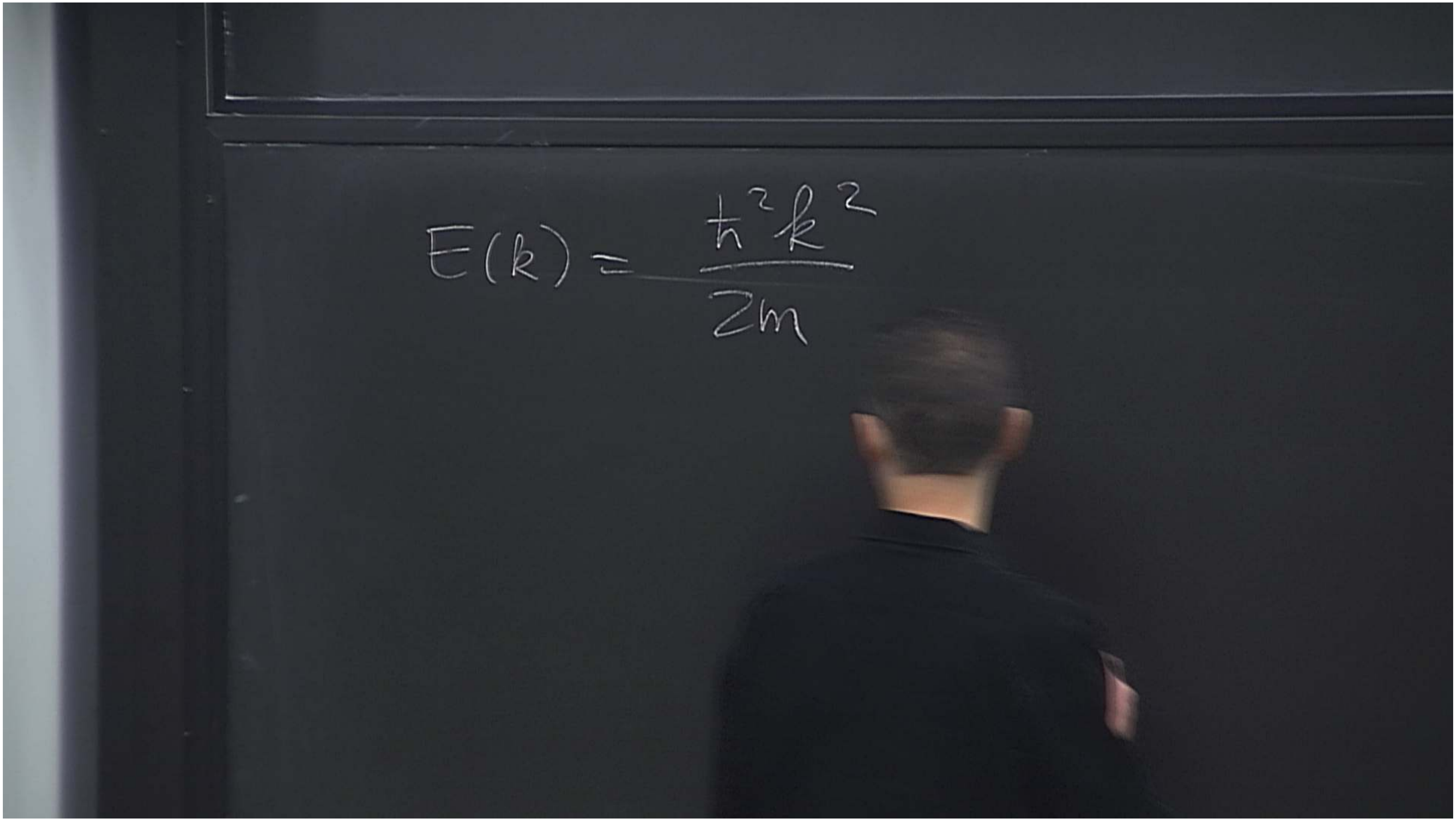
Hexagonal (triangular) lattice

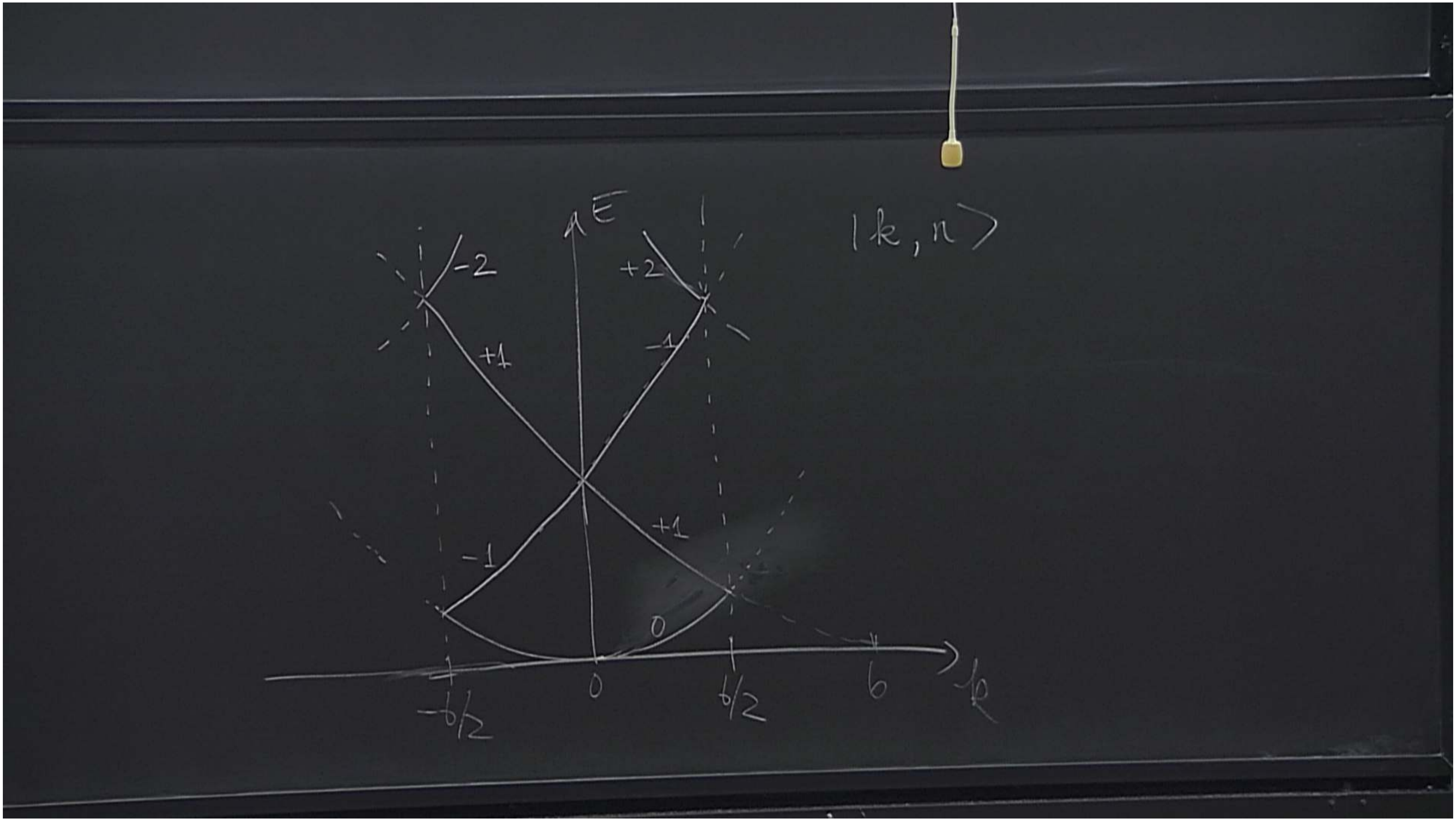
$\vec{a}_2 = \left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right)a$

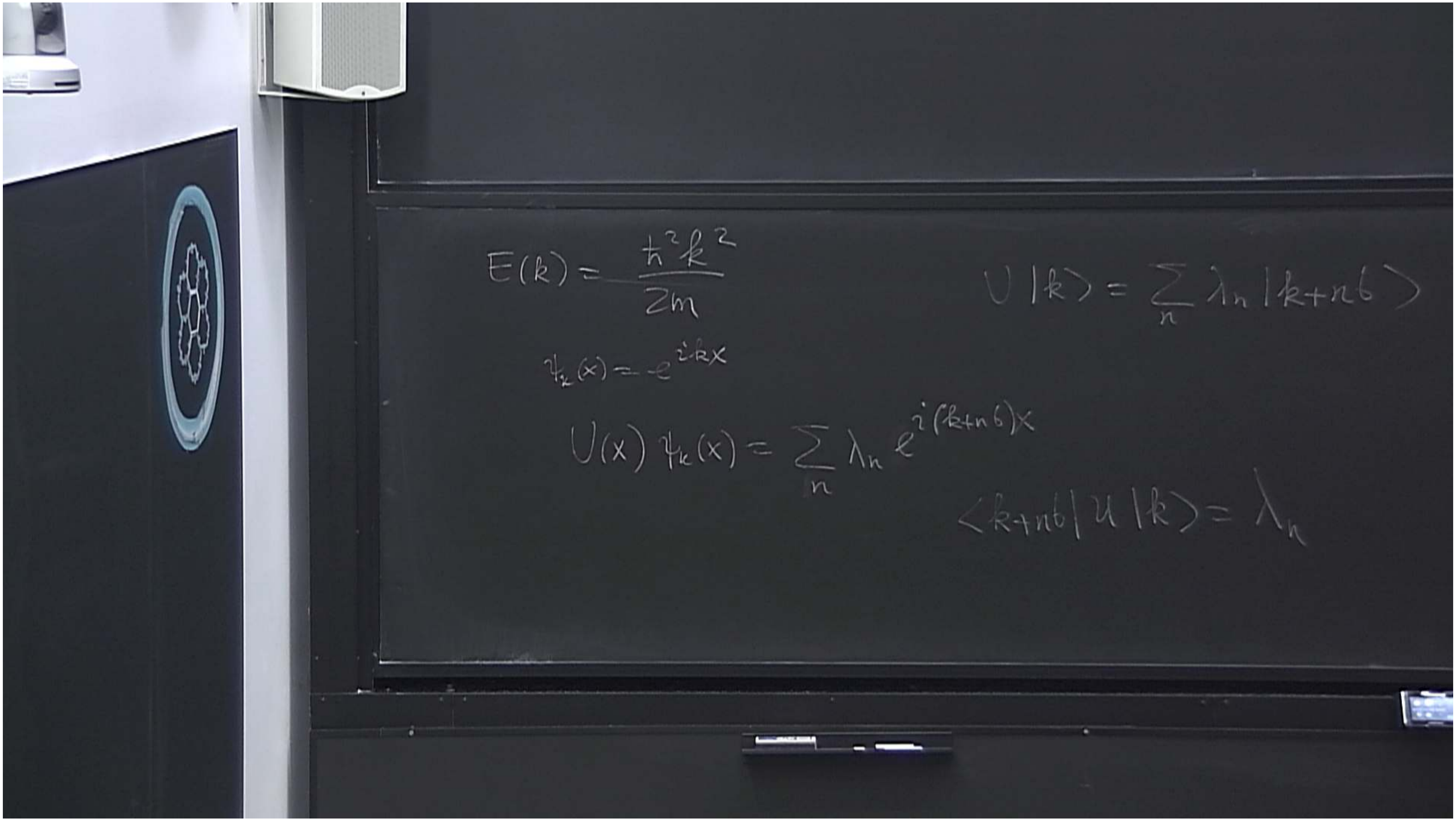
$\vec{a}_1 = (1,0)a$

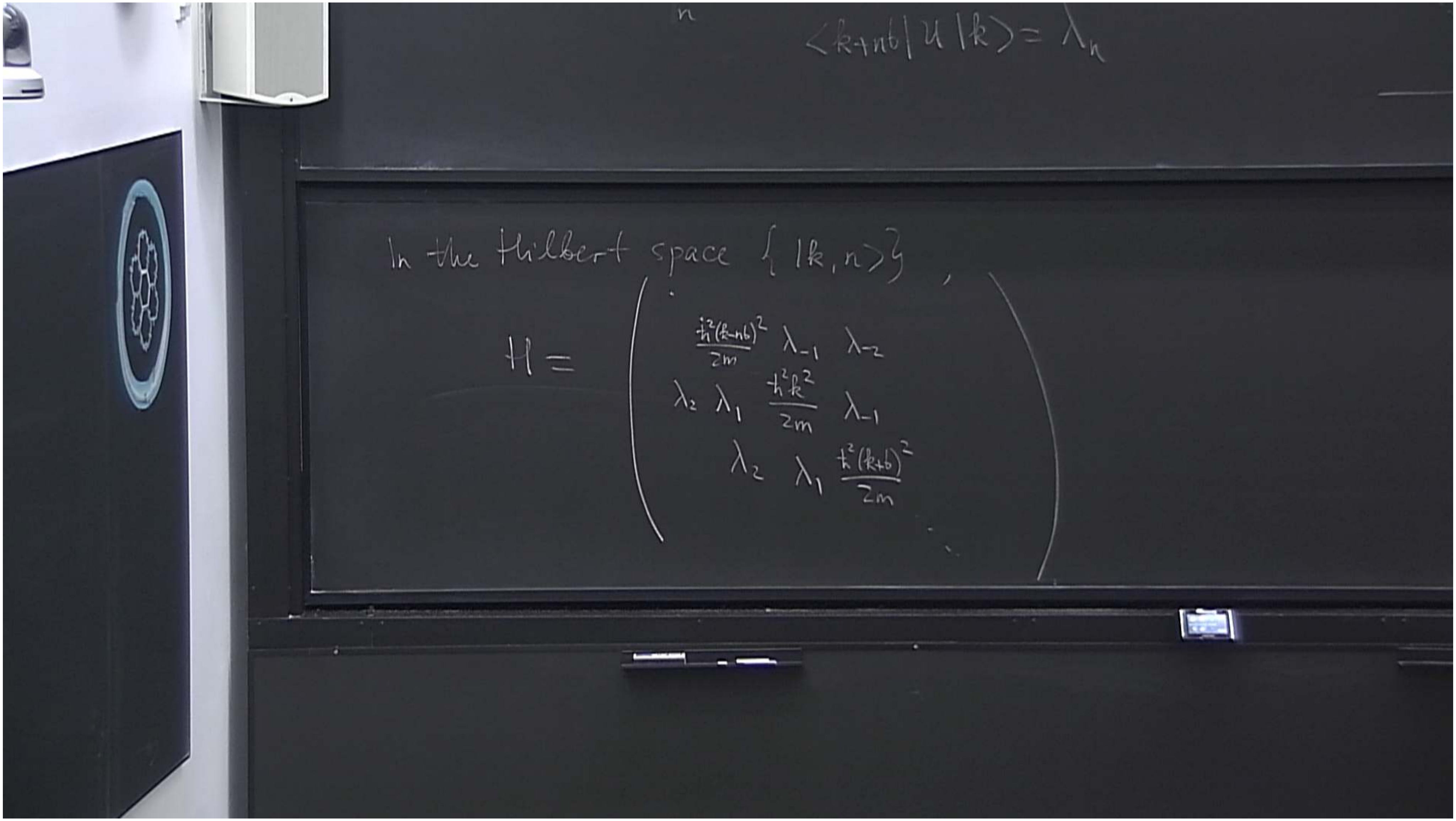

Electron in a periodic potential $U(x) = U(x+a)$, a is the lattice period.
$H\psi(x) = E\psi(x)$, $H = \frac{p^2}{2m} + U(x)$, $p = -i\hbar\frac{d}{dx}$
Weak potential.
If $U=0$ then $\psi(x) = e^{ikx}$, $E = \hbar^2 k^2/2m$.
$U|k\rangle = \sum_n \lambda_n |k+nb\rangle$
$U(x) = \sum_n \lambda_n e^{inbx}$, $b = 2\pi/a$, $n \in \mathbb{Z}$, $\lambda_n^* = \lambda_{-n}$
$\hbar k$ not a conserved quantity
$-b$
$+b$
$-b$
0
k
b
k



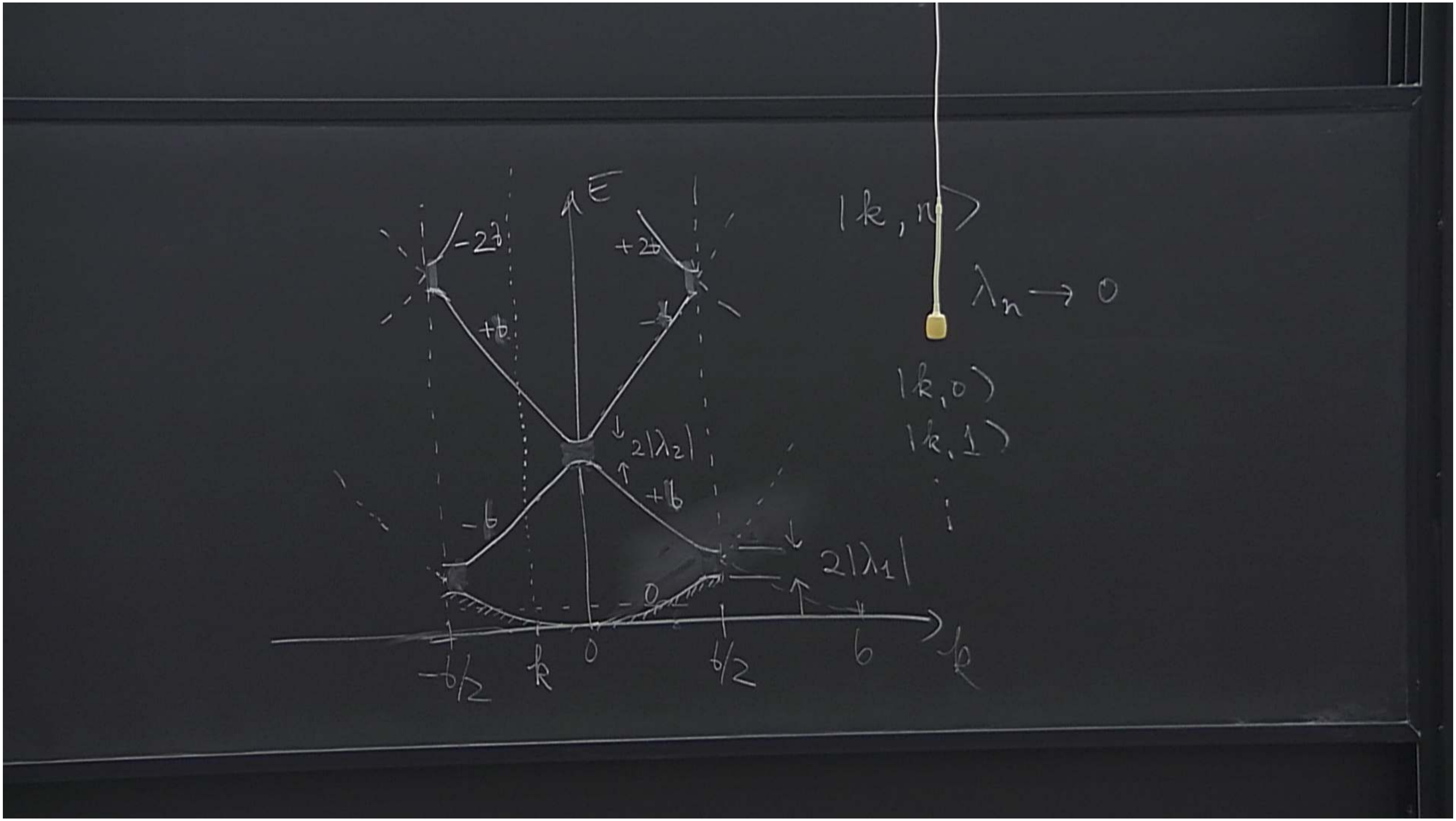

$E(k) = \frac{\hbar^2 k^2}{2m}$


E
$|k, n\rangle$
−2
+2
+1
−1
−1
+1
0
$-b/2$
0
$b/2$
b
k

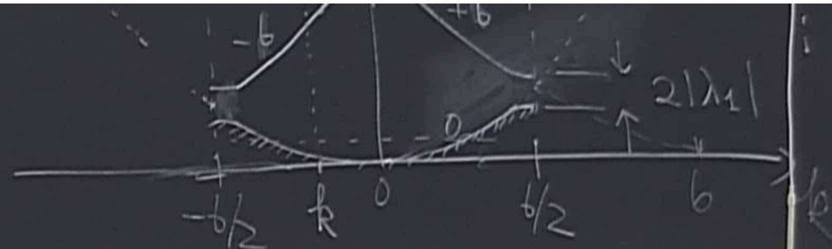

$E(k) = \frac{\hbar^2 k^2}{2m}$
$U|k\rangle = \sum_n \lambda_n |k+nb\rangle$
$\psi_k(x) = e^{ikx}$
$U(x)\,\psi_k(x) = \sum_n \lambda_n e^{i(k+nb)x}$
$\langle k+nb|U|k\rangle = \lambda_n$



n
$\langle k+nb | U | k \rangle = \lambda_n$
In the Hilbert space $\{ |k,n\rangle \}$,
$H = \begin{pmatrix} \ddots & & & & \\ & \frac{\hbar^2(k-nb)^2}{2m} & \lambda_{-1} & \lambda_{-2} & \\ \lambda_2 & \lambda_1 & \frac{\hbar^2 k^2}{2m} & \lambda_{-1} & \\ & \lambda_2 & \lambda_1 & \frac{\hbar^2(k+b)^2}{2m} & \\ & & & & \ddots \end{pmatrix}$


E
-2b
+2b
+b
-b
2|λ2|
+b
-b
2|λ1|
0
-b/2
k
0
b/2
b
k
|k, n⟩
λn → 0
|k, 0⟩
|k, 1⟩

$u|k\rangle = \lambda_n$



Direct lattice of atoms $\cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \xleftrightarrow{a} \cdot$

Wavenumbers $\Delta k = nb,\ b = \frac{2\pi}{a}$ $\quad -b \quad 0 \quad b \quad 2b$

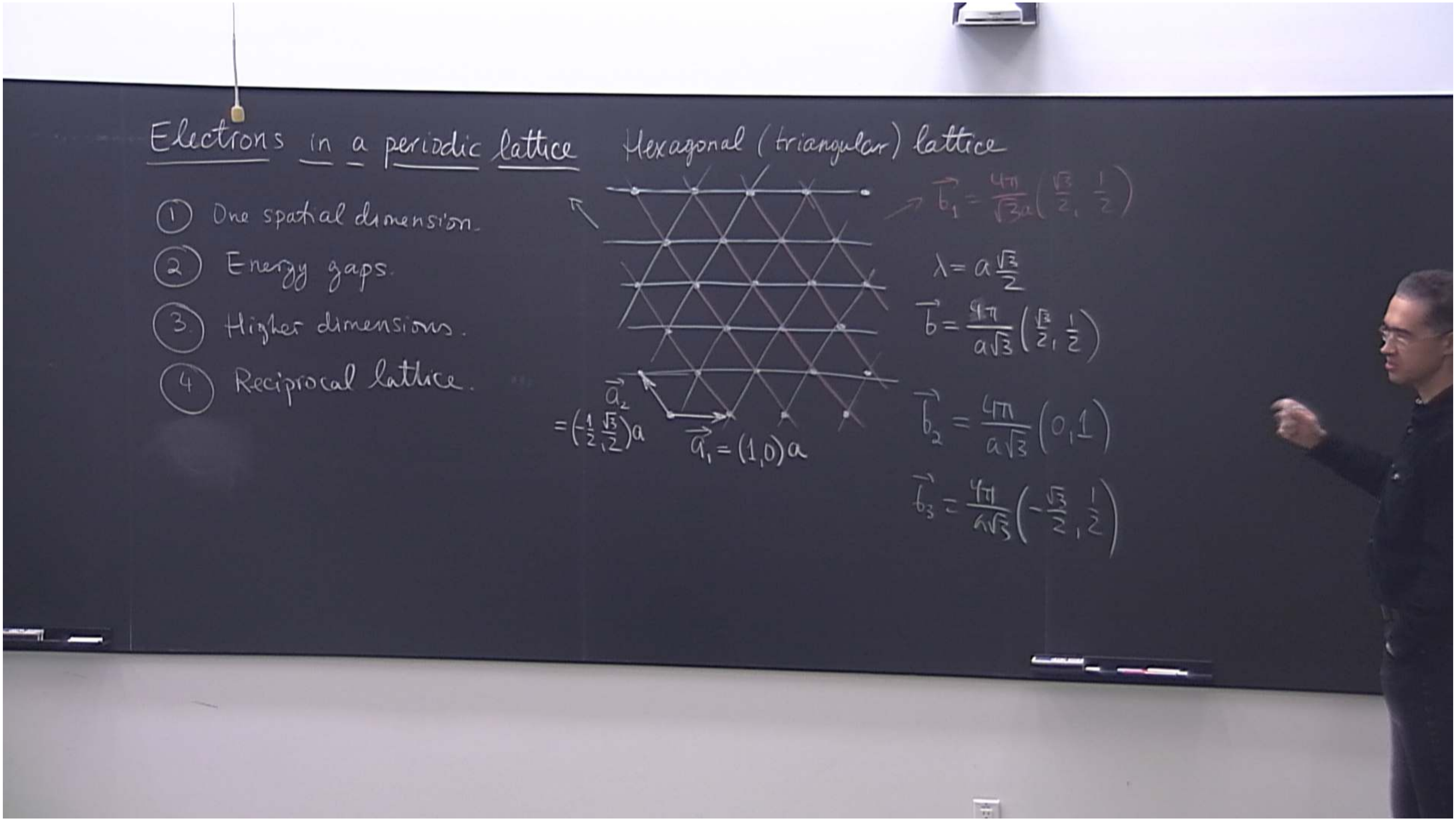
Reciprocal lattice

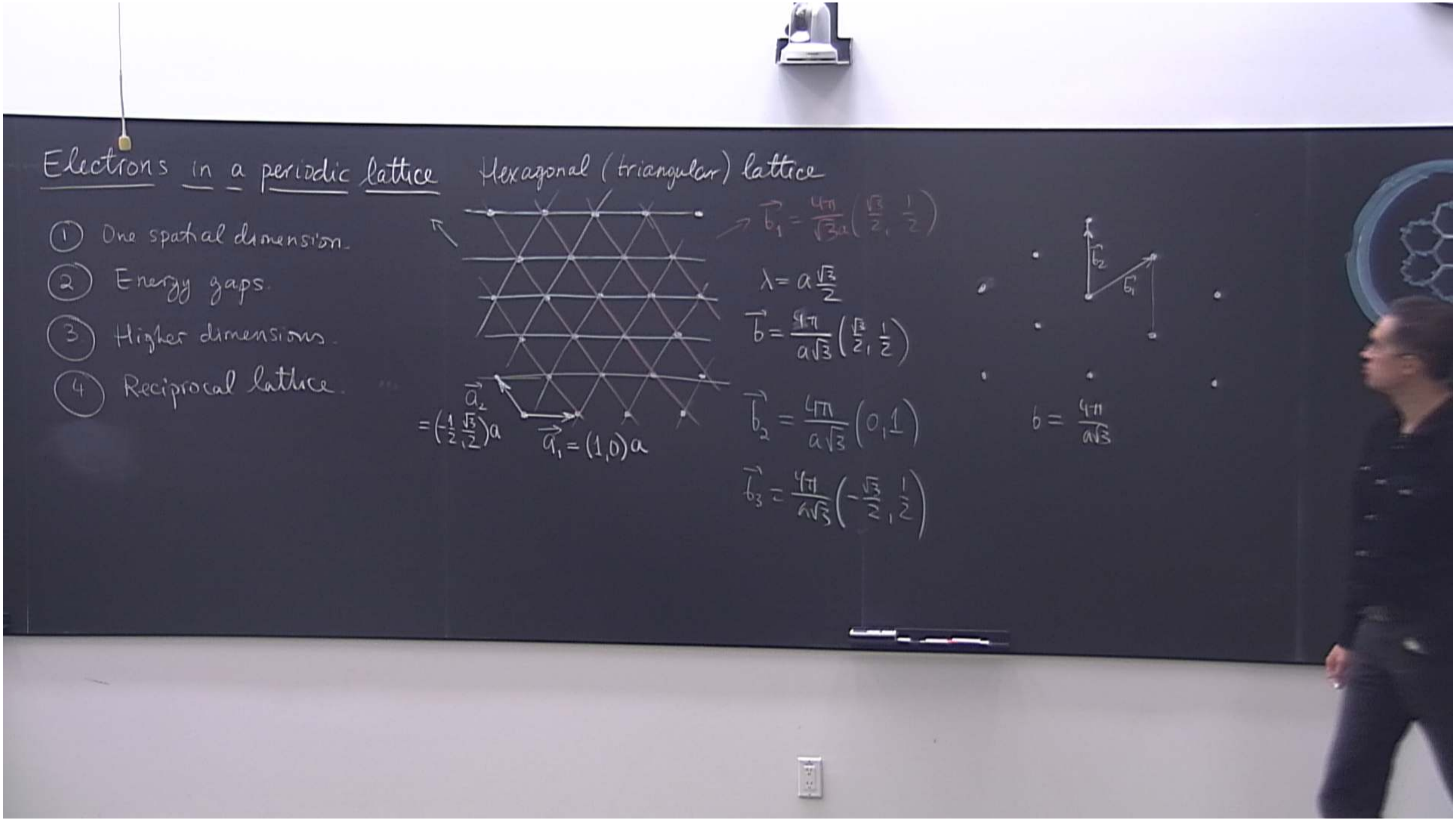
$$ab = 2\pi$$

$$\mathcal{U}(\vec r+\vec a_1) = \mathcal{U}(\vec r) = \mathcal{U}(\vec r+\vec a_2) = \mathcal{U}(\vec r+\vec a), \quad \vec a = n_1\vec a_1 + n_2\vec a_2, \quad n_1, n_2 \in \mathbb{Z}.$$

$$\mathcal{U}(\vec r) = \sum_{\vec b} \lambda_{\vec b}\, e^{i\vec b\cdot\vec r}, \quad \lambda^*_{\vec b} = \lambda_{-\vec b}$$

$$\tilde{\mathcal{U}}(\vec k) = \int \mathcal{U}(\vec r)\, e^{-i\vec k\cdot\vec r}\, d^2r = \sum_{\vec b}\int \lambda_{\vec b}\, e^{i\vec b\cdot\vec r - i\vec k\cdot\vec r}\, d^2r = \sum_{\vec b} (2\pi)^2\, \delta(\vec k-\vec b)\, \lambda_{\vec b}$$


Electrons in a periodic lattice
1 One spatial dimension.
2 Energy gaps.
3 Higher dimensions.
4 Reciprocal lattice.
Hexagonal (triangular) lattice
$\vec{a}_2 = \left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right)a$
$\vec{a}_1 = (1,0)a$
$\vec{b}_1 = \frac{4\pi}{\sqrt{3}a}\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$
$\lambda = a\frac{\sqrt{3}}{2}$
$\vec{b} = \frac{4\pi}{a\sqrt{3}}\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$
$\vec{b}_2 = \frac{4\pi}{a\sqrt{3}}(0,1)$
$\vec{b}_3 = \frac{4\pi}{a\sqrt{3}}\left(-\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$


Electrons in a periodic lattice
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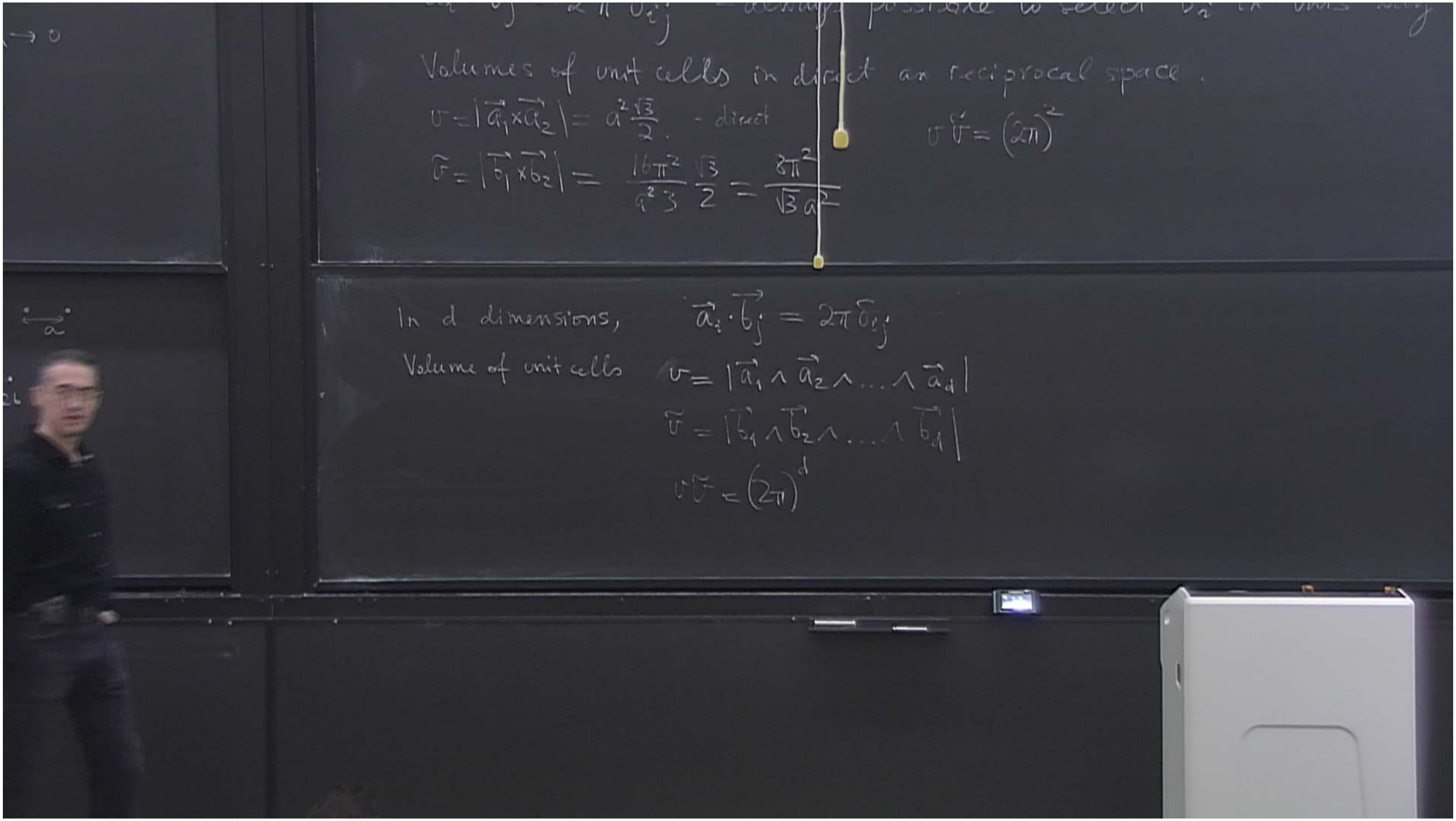
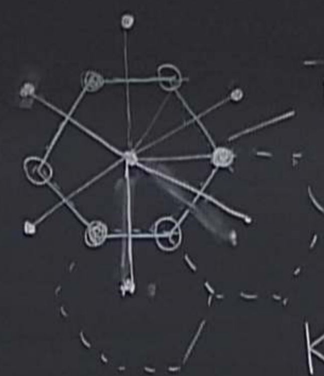
Hexagonal (triangular) lattice
$\vec{a}_2 = (-\frac{1}{2}, \frac{\sqrt{3}}{2})a$
$\vec{a}_1 = (1,0)a$
$\vec{b}_1 = \frac{4\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{2}, \frac{1}{2})$
$\lambda = a\frac{\sqrt{3}}{2}$
$\vec{b} = \frac{4\pi}{a\sqrt{3}}(\frac{\sqrt{3}}{2}, \frac{1}{2})$
$\vec{b}_2 = \frac{4\pi}{a\sqrt{3}}(0,1)$
$\vec{b}_3 = \frac{4\pi}{a\sqrt{3}}(-\frac{\sqrt{3}}{2}, \frac{1}{2})$
$\vec{b}_2$
$\vec{b}_1$
$b = \frac{4\pi}{a\sqrt{3}}$


Volumes of unit cells in direct an reciprocal space.
$v = |\vec{a}_1 \times \vec{a}_2| = a^2 \frac{\sqrt{3}}{2}$ - direct
$\tilde{v} = |\vec{b}_1 \times \vec{b}_2| = \frac{16\pi^2}{a^2 3} \frac{\sqrt{3}}{2} = \frac{8\pi^2}{\sqrt{3} a^2}$
$v \tilde{v} = (2\pi)^2$
In d dimensions, $\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$
Volume of unit cells $v = |\vec{a}_1 \wedge \vec{a}_2 \wedge \ldots \wedge \vec{a}_d|$
$\tilde{v} = |\vec{b}_1 \wedge \vec{b}_2 \wedge \ldots \wedge \vec{b}_d|$
$v \tilde{v} = (2\pi)^d$

$$\vec{K} = \left(\frac{4\pi}{3a}, 0\right)$$

$\vec{K}'$

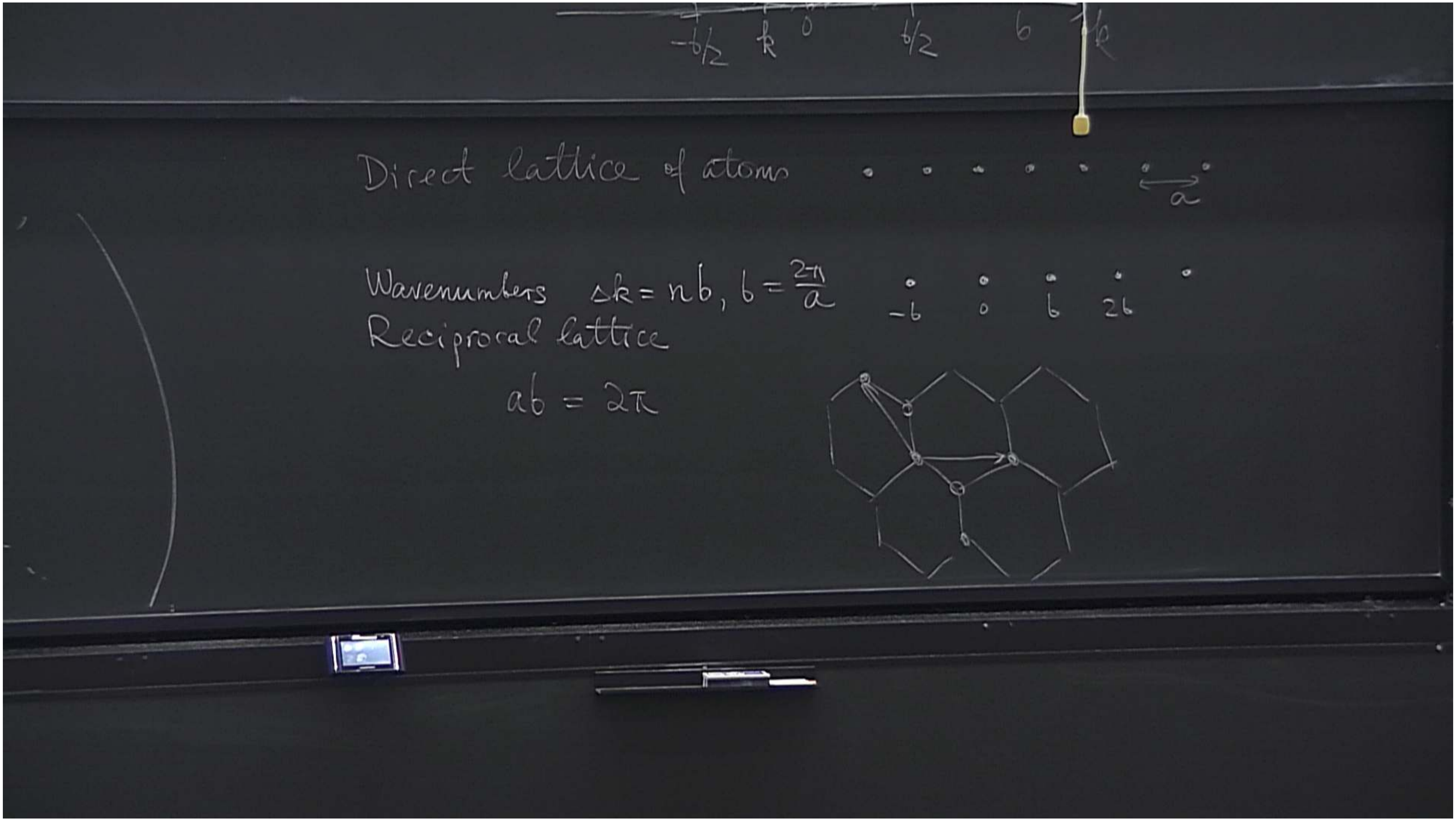


$$\vec{K} = (K, 0)$$

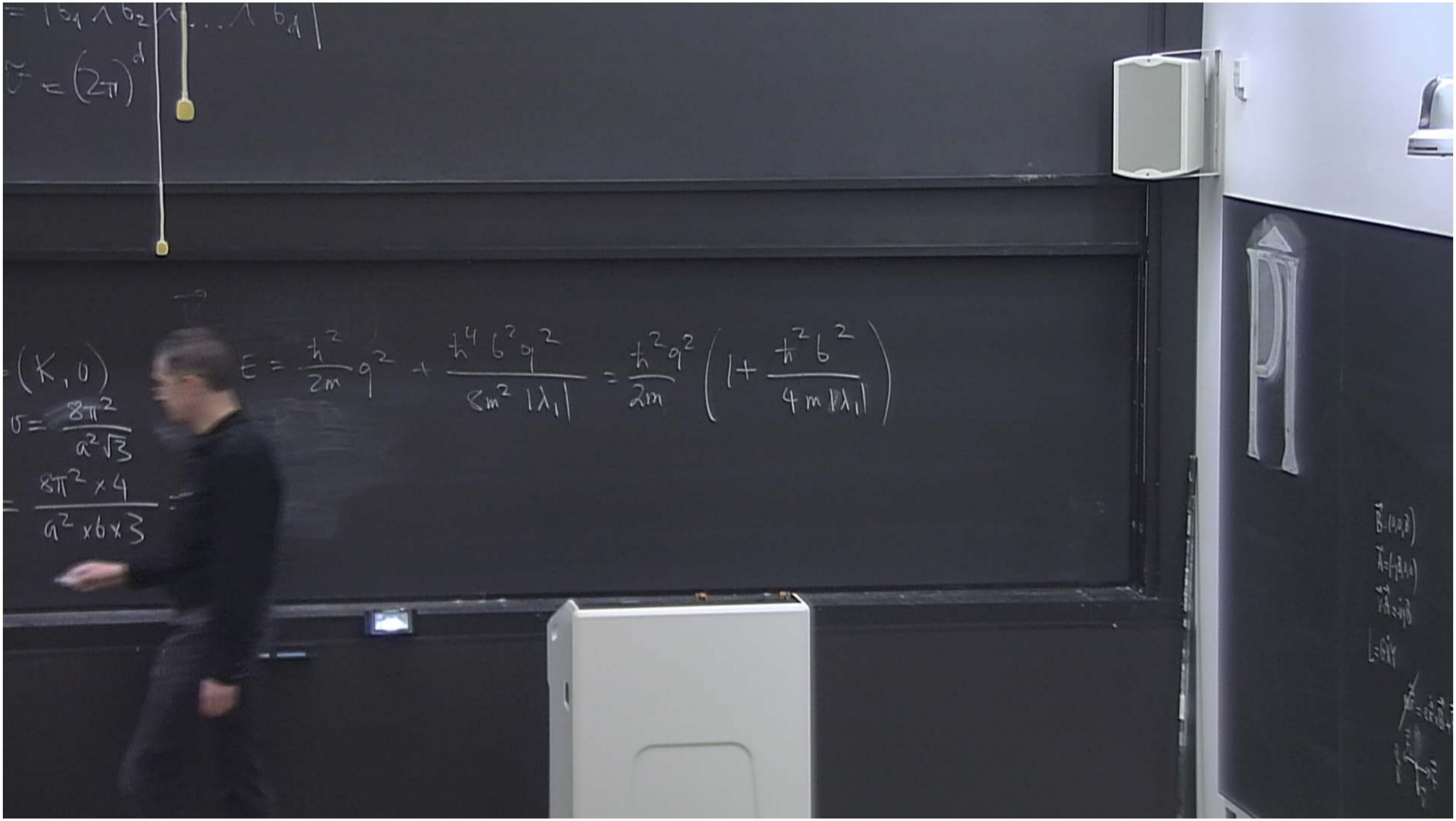
$$\vec{K}' = -\vec{K}$$

$$\sigma = \frac{8\pi^2}{a^2\sqrt{3}} = 6 \times \frac{1}{2} K^2 \frac{\sqrt{3}}{2},$$

$$K^2 = \frac{8\pi^2 \times 4}{a^2 \times 6 \times 3} = \frac{16\pi^2}{9a^2}$$



-b/2 k 0 b/2 b k
Direct lattice of atoms
a
Wavenumbers Δk = nb, b = 2π/a
-b 0 b 2b
Reciprocal lattice
ab = 2π


(K, 0)
σ = 8π²/a²√3
= 8π²×4/a²×6×3
E = ħ²/2m q² + ħ⁴b²q²/8m²|λ₁| = ħ²q²/2m (1 + ħ²b²/4m|λ₁|)