

Title: Condensed Matter 101 - Lecture 3

Date: Aug 29, 2012 10:30 AM

URL: <http://pirsa.org/12080034>

Abstract:

Today

(*) Some information
about crystal lattices

(**) Bloch's theorem

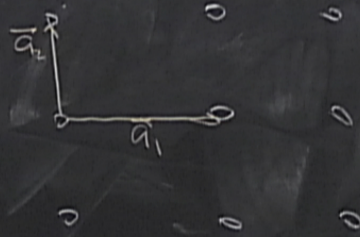
Some information about crystal lattices

Bravais lattice (BL) is the lattice in which the neighborhood of each site is the same

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \quad (n_i \in \mathbb{Z})$$

$\vec{a}_i$ - primitive vectors

which are linearly independent,



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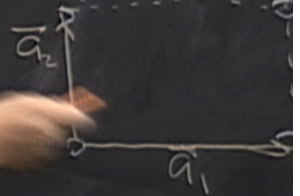
$\vec{a}_i$ - the primitive vectors

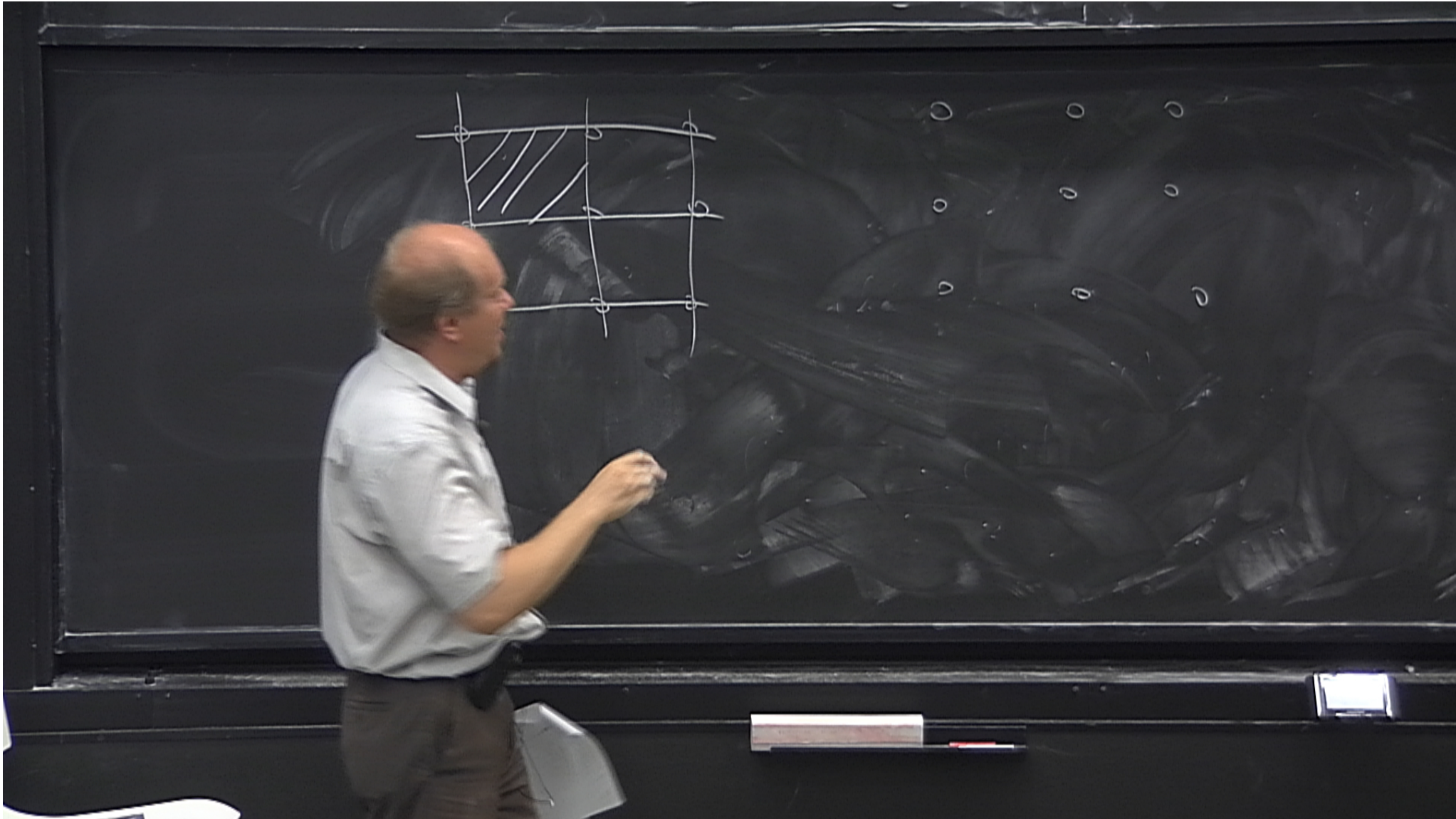
while $\vec{a}_i$ are linearly independent,
their choice is not unique

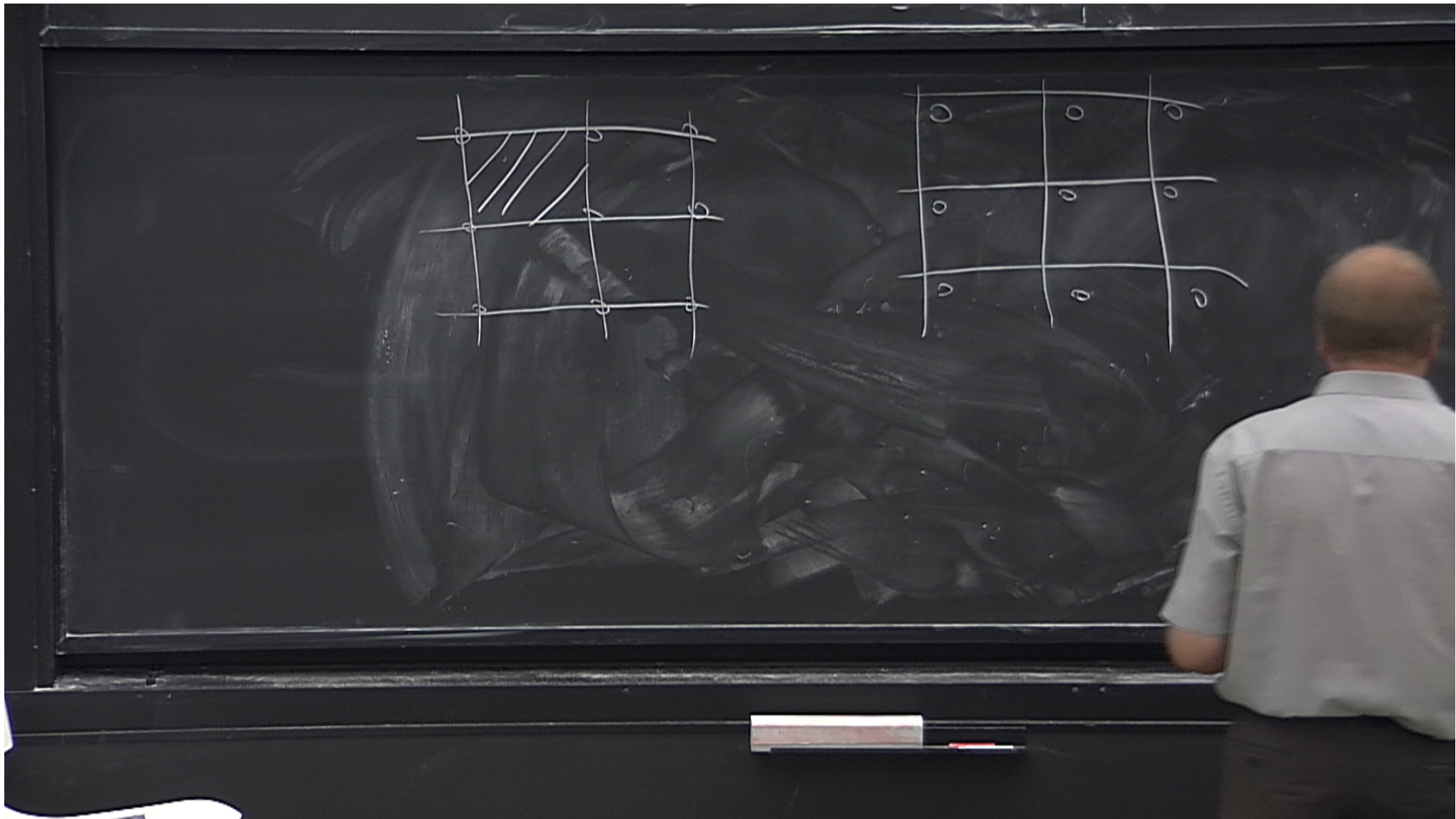


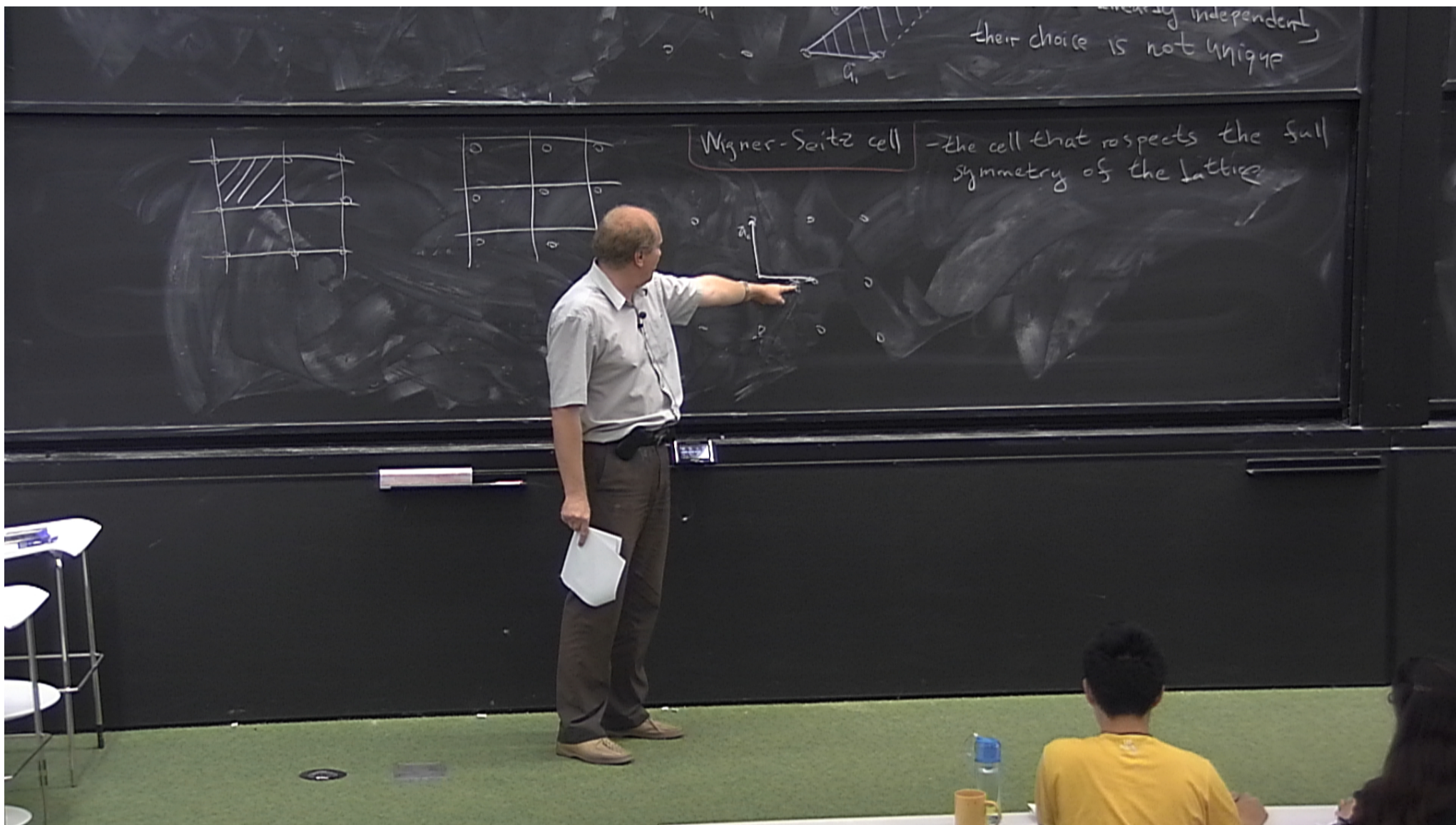
Unit (primitive) cell volume
of space which is transported
by $\vec{R} \in BL$ fills space
with no voids

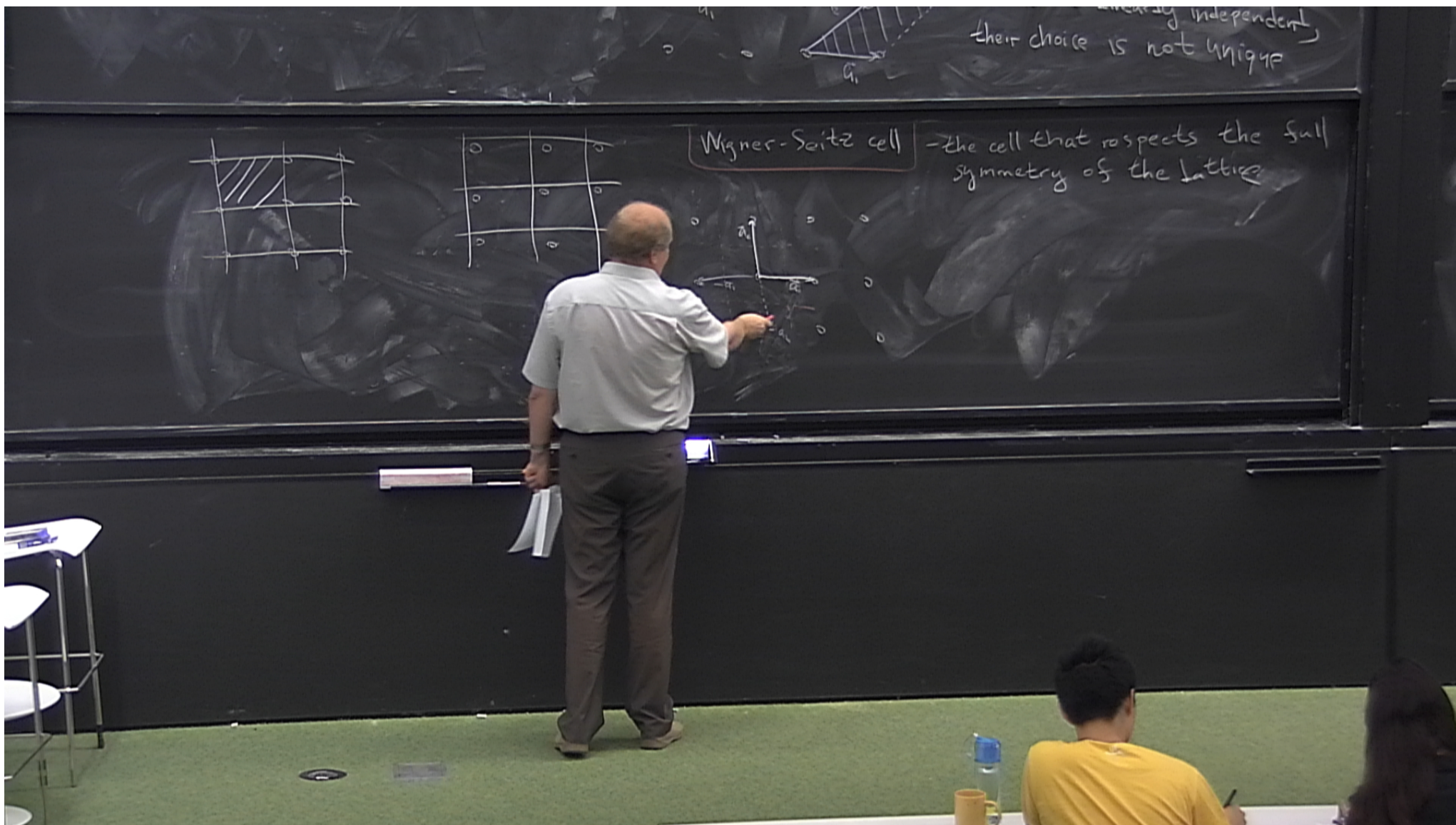
Some information
Bravais Lattice (BL)
Site is the same

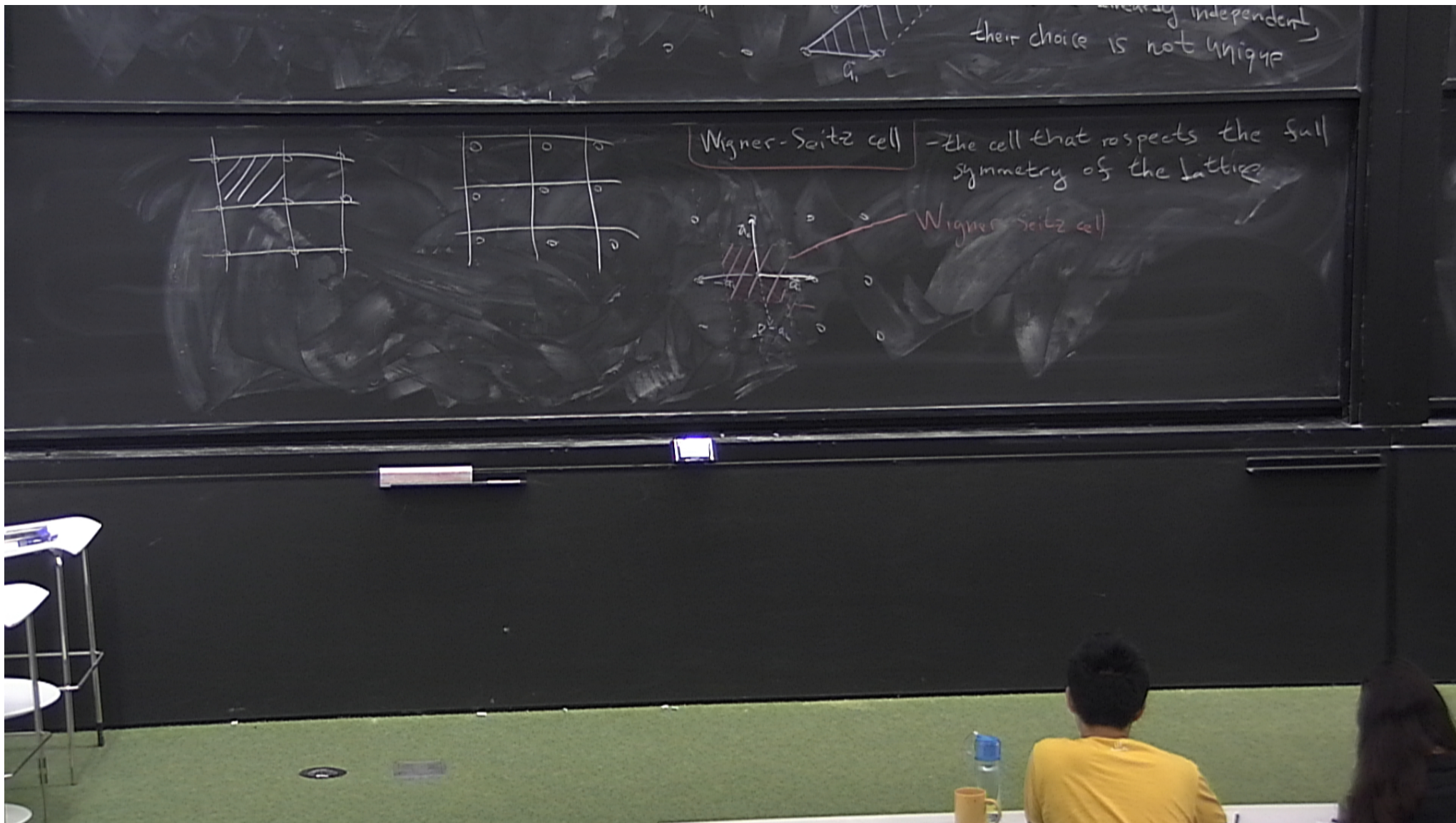






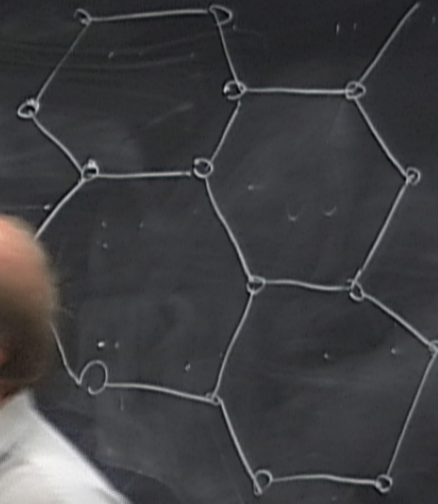


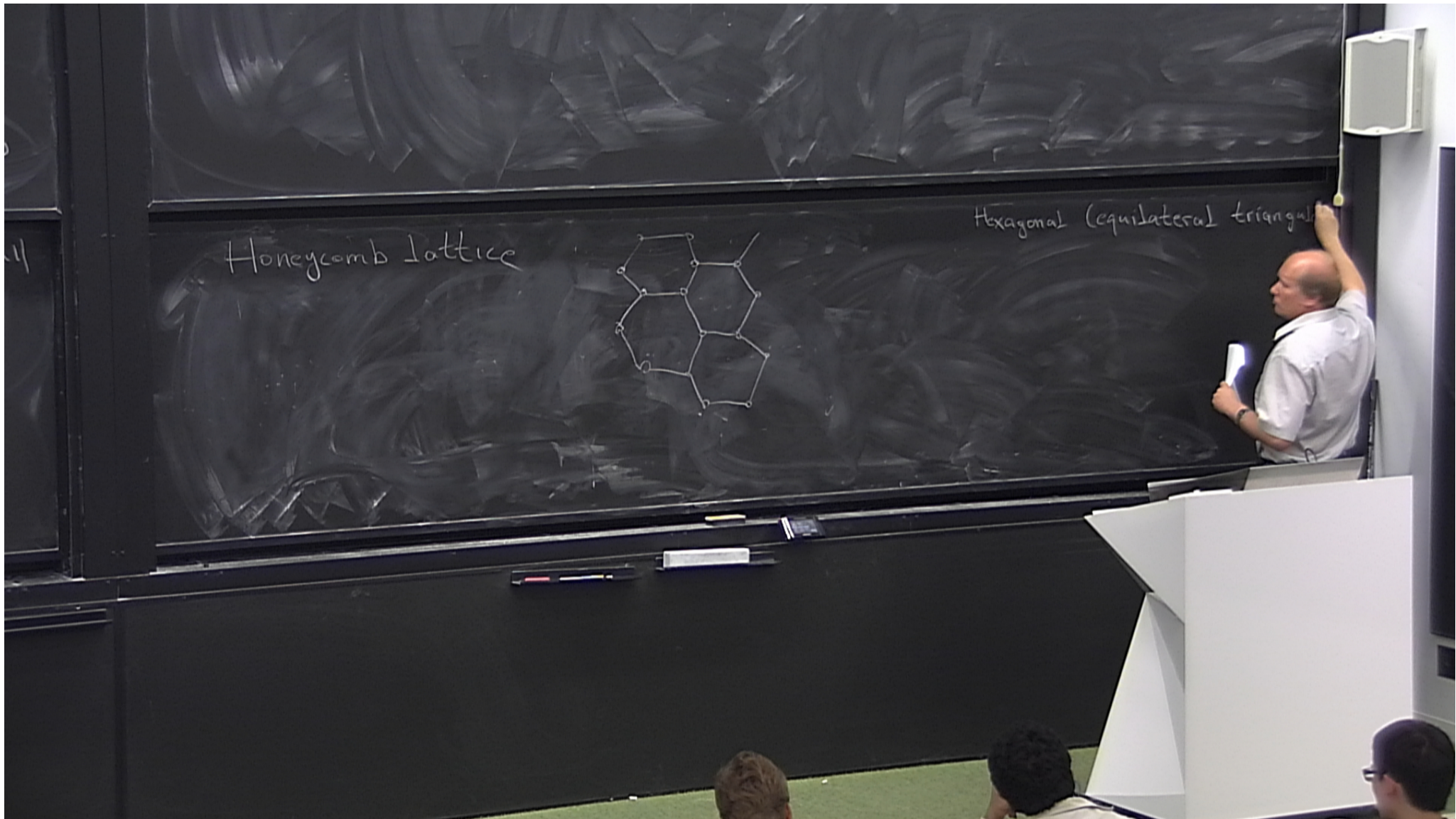


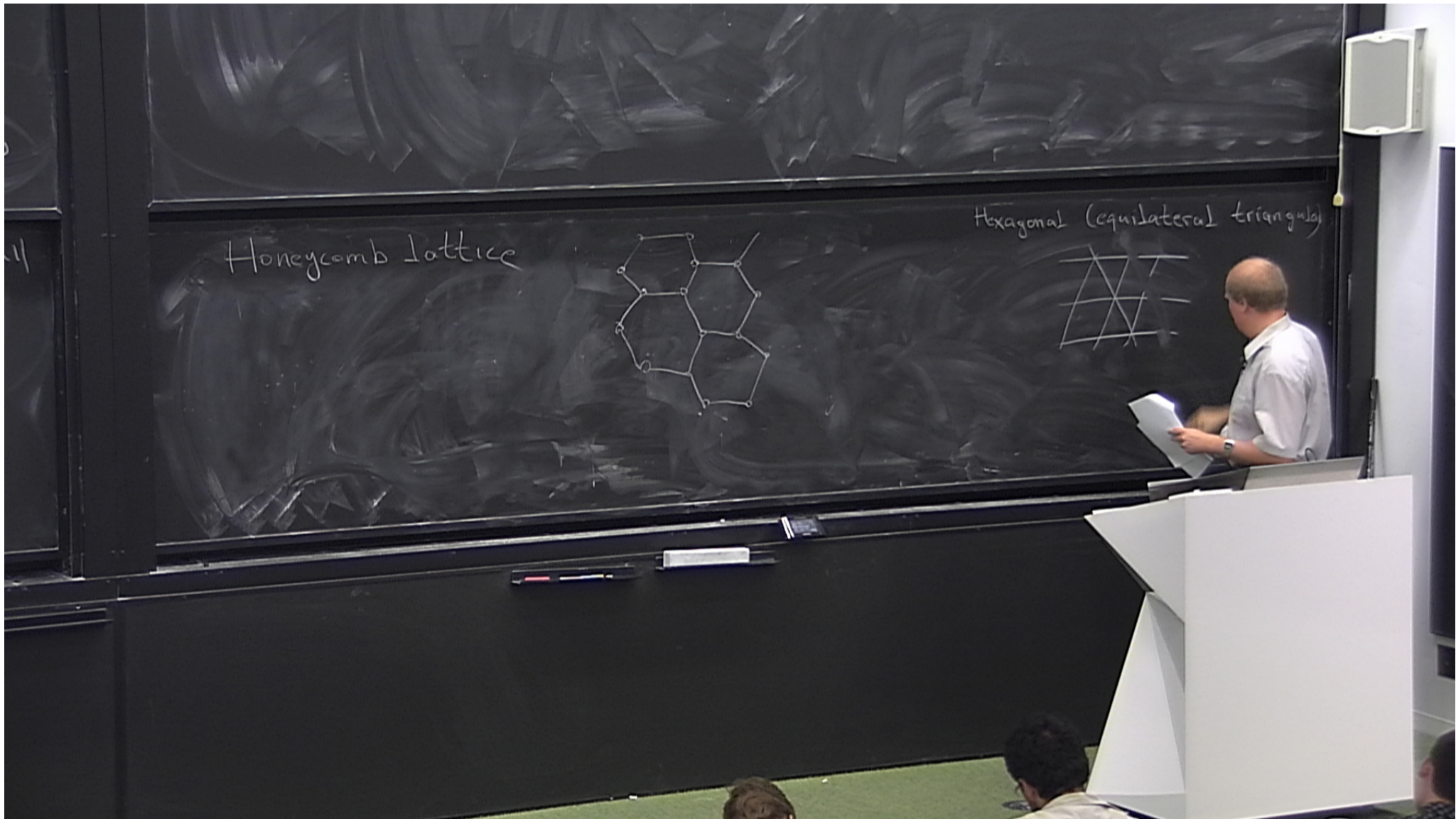


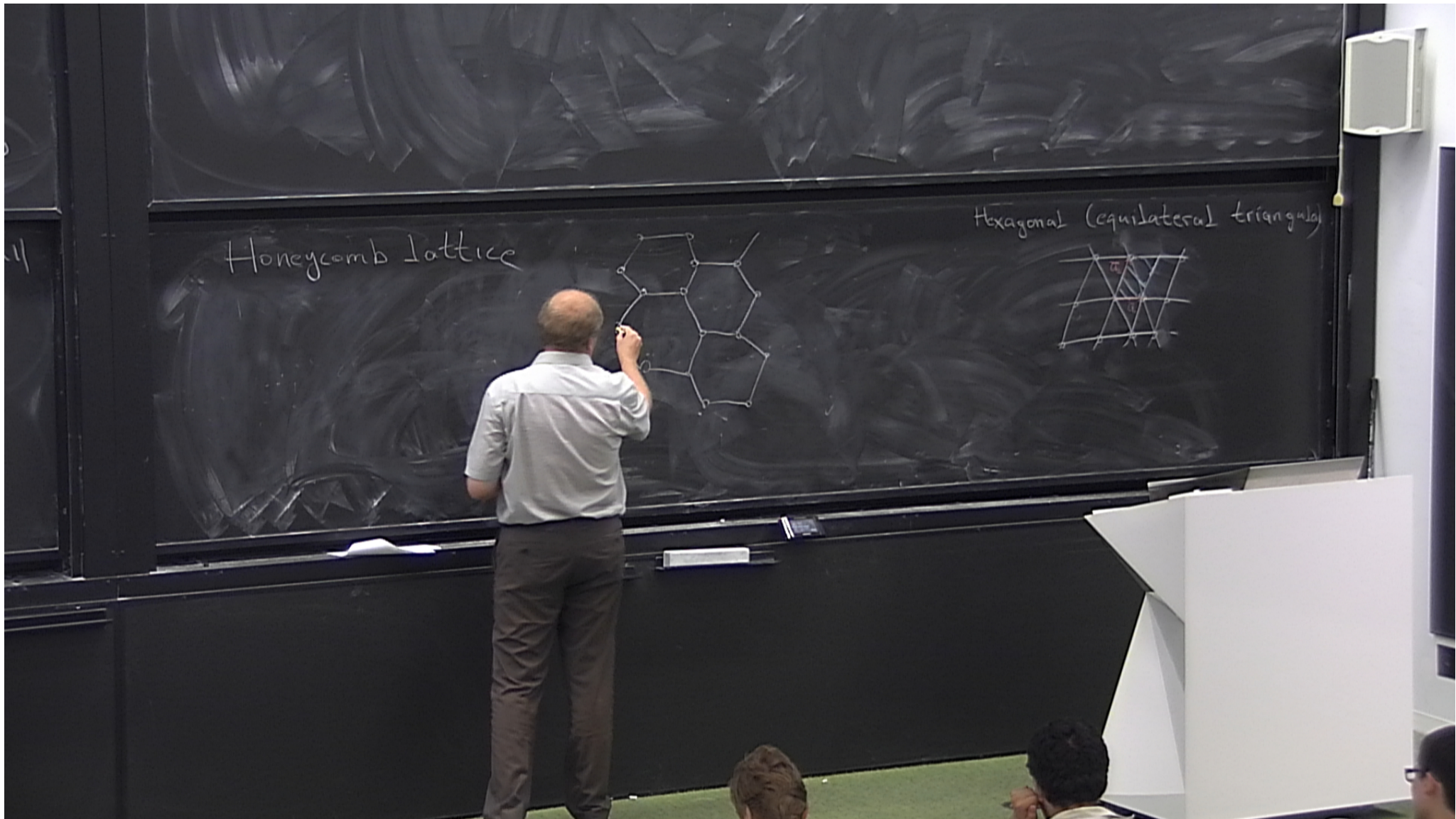
Honeycomb 1

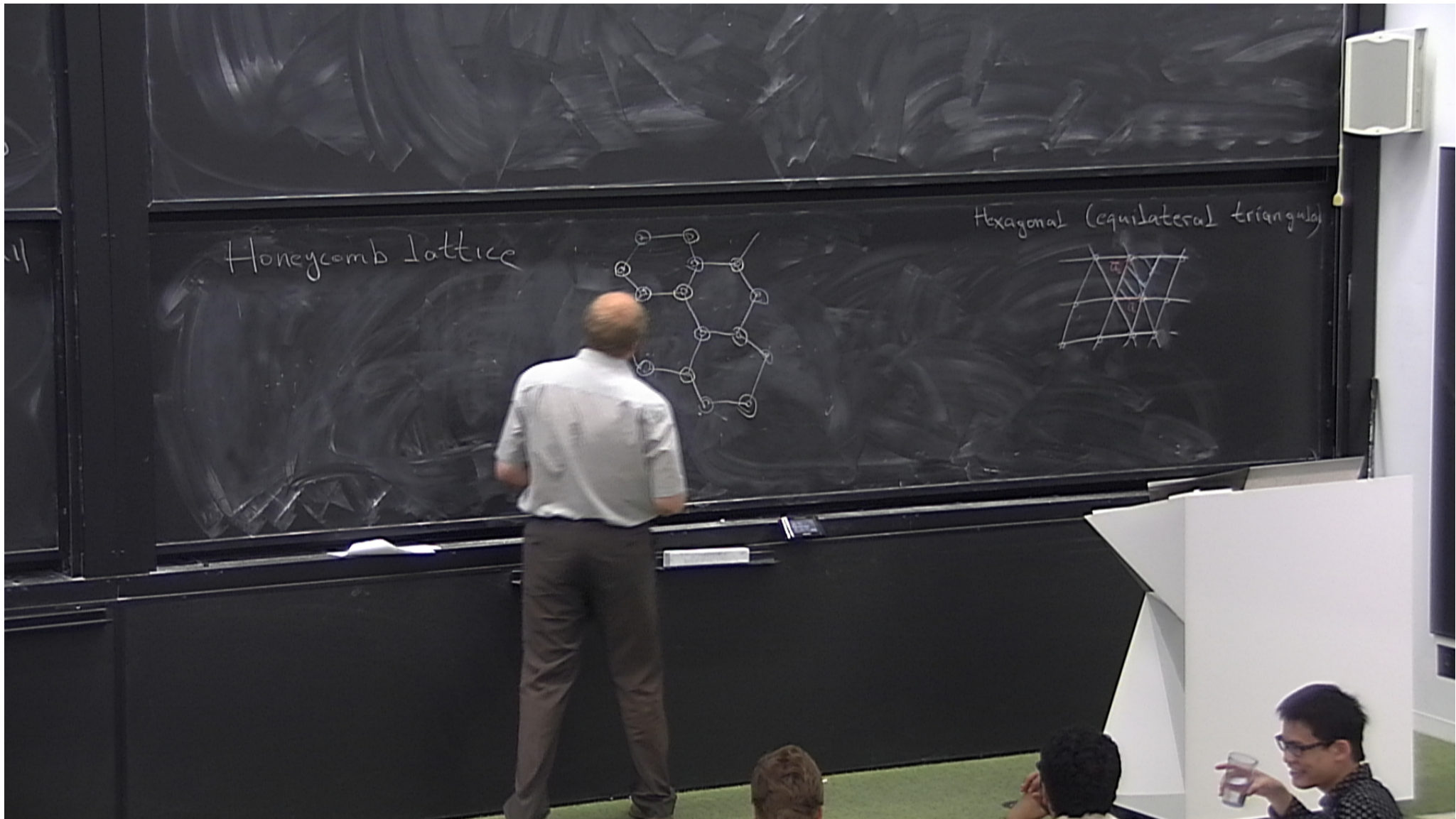
Honeycomb Lattice



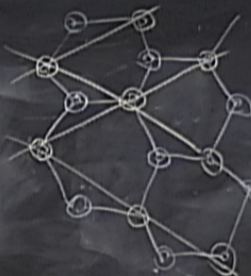








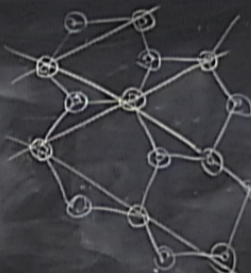
Honeycomb lattice
is the lattice with
the basis



Hexagonal (equilateral triangular)



Honeycomb lattice
is the lattice with
the basis
(Ex: Graphene)



Hexagonal (equilateral triangular)



Reciprocal Lattice, first Brillouin zone
vectors $\mathbf{K}$ constitute the RL if a

Reciprocal Lattice, first Brillouin zone

Vectors $\vec{K}$ constitute the RL if for a given BL ($\vec{R} = \text{BL}$), one has $e^{i\vec{K} \cdot \vec{R}} = 1$

RL is also BL in momentum space

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RL is also BL in momentum space

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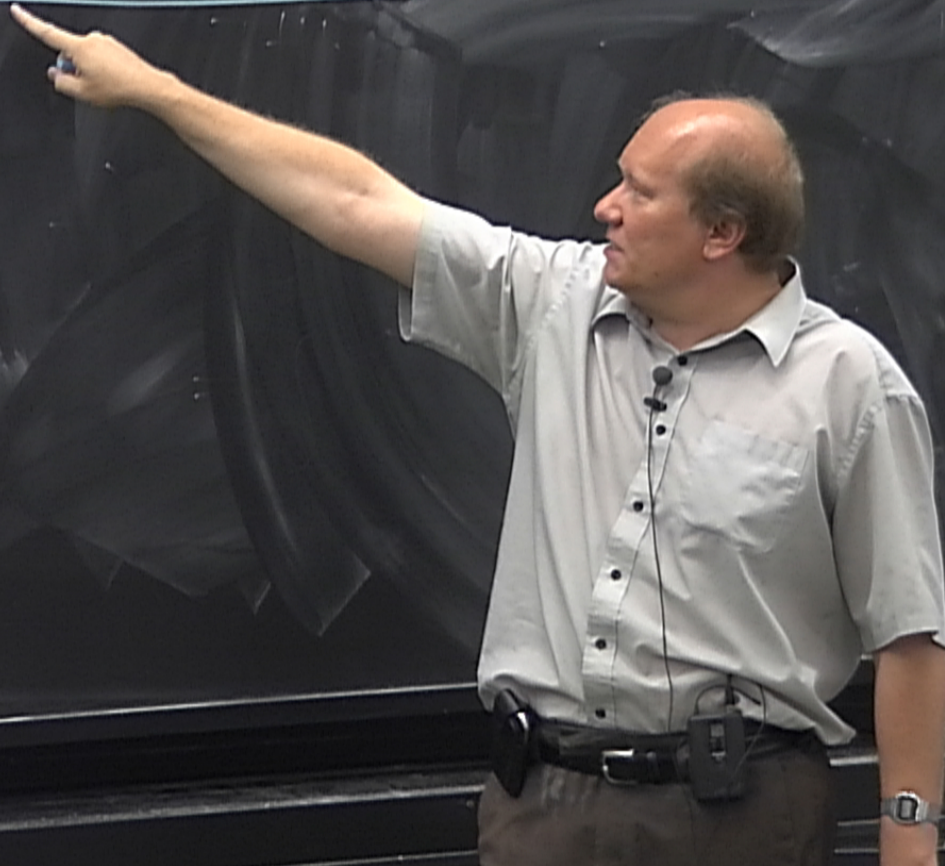
Reciprocal Lattice, first Brillouin zone

Vectors $\vec{K}$ constitute the RL if for a given BL ($\vec{R}$ = BL), one has $e^{i\vec{K} \cdot \vec{R}} = 1$

RL is also BL in momentum space, $\vec{K} = \sum_{i=1}^d k_i \vec{b}_i$, $\vec{b}_i$ form the basis
 $k_i \in \mathbb{Z}$

(Ex. Graphene)

$$\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}$$

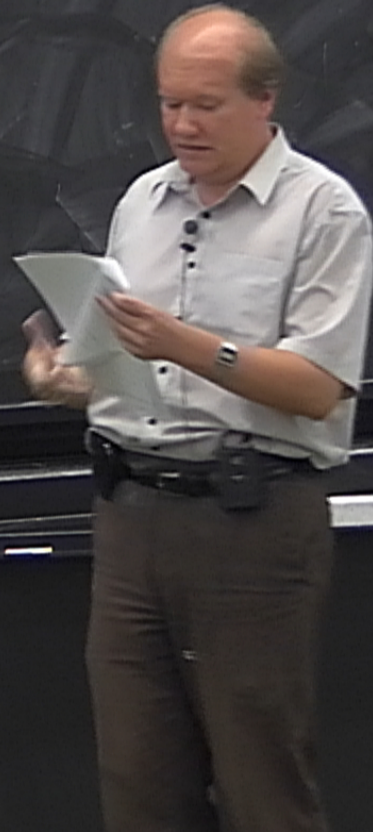


(Ex: Graphene)

$$\boxed{\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}} \quad \vec{R} = \sum_{\vec{i}} n_i \vec{a}_i, \quad \vec{K} \cdot \vec{R} = 2\pi \sum_{\vec{i}} n_i k_i$$

(Ex: Graphene)

$$\boxed{\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}} \quad \vec{R} = \sum_{\vec{n}} n_i \vec{a}_i, \quad \vec{K} \cdot \vec{R} = 2\pi \sum_{\vec{n}} n_i k_i \Rightarrow \exp(i\vec{K} \cdot \vec{R}) = 1$$



in zone

for a given BL ($\vec{R} = BL$), one has

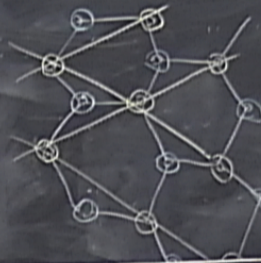
$$e^{i\vec{K} \cdot \vec{R}} = 1$$

$$\vec{K} = \sum_i k_i \vec{b}_i, \quad \vec{b}_i \text{ form the basis}$$

$k_i \in \mathbb{Z}$

$\downarrow$ RL vector

Honeycomb lattice
is the lattice with
the basis
(Ex: Graphene)



Hexagonal (equilateral triangular)

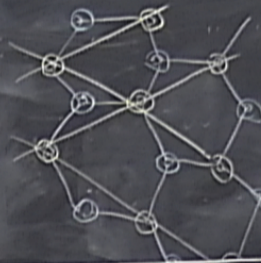


$$\boxed{\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}} \quad \vec{R} = \sum_{\vec{n}} n \cdot \vec{a}_i \quad \vec{K} \cdot \vec{R} = 2\pi \sum_{\vec{n}} n \cdot \vec{k} \Rightarrow \exp(i \vec{K} \cdot \vec{R}) = 1$$

(1D)

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

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$$|\vec{b}_i \cdot \vec{a}_j| = 2\pi \delta_{ij} \quad \vec{R} = \sum_{\vec{n}} n \cdot \vec{a}_i \quad \vec{K} \cdot \vec{R} = 2\pi \sum_{\vec{n}} n \cdot \vec{k} \Rightarrow \exp(i \vec{K} \cdot \vec{R}) = 1$$

(1D)

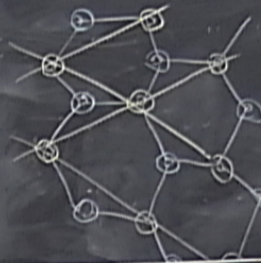
$$\vec{a} = a\hat{x}$$

RL

$$\vec{b} = \frac{2\pi}{a}\hat{x}$$

3D

Honeycomb lattice
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Hexagonal (equilateral triangular)

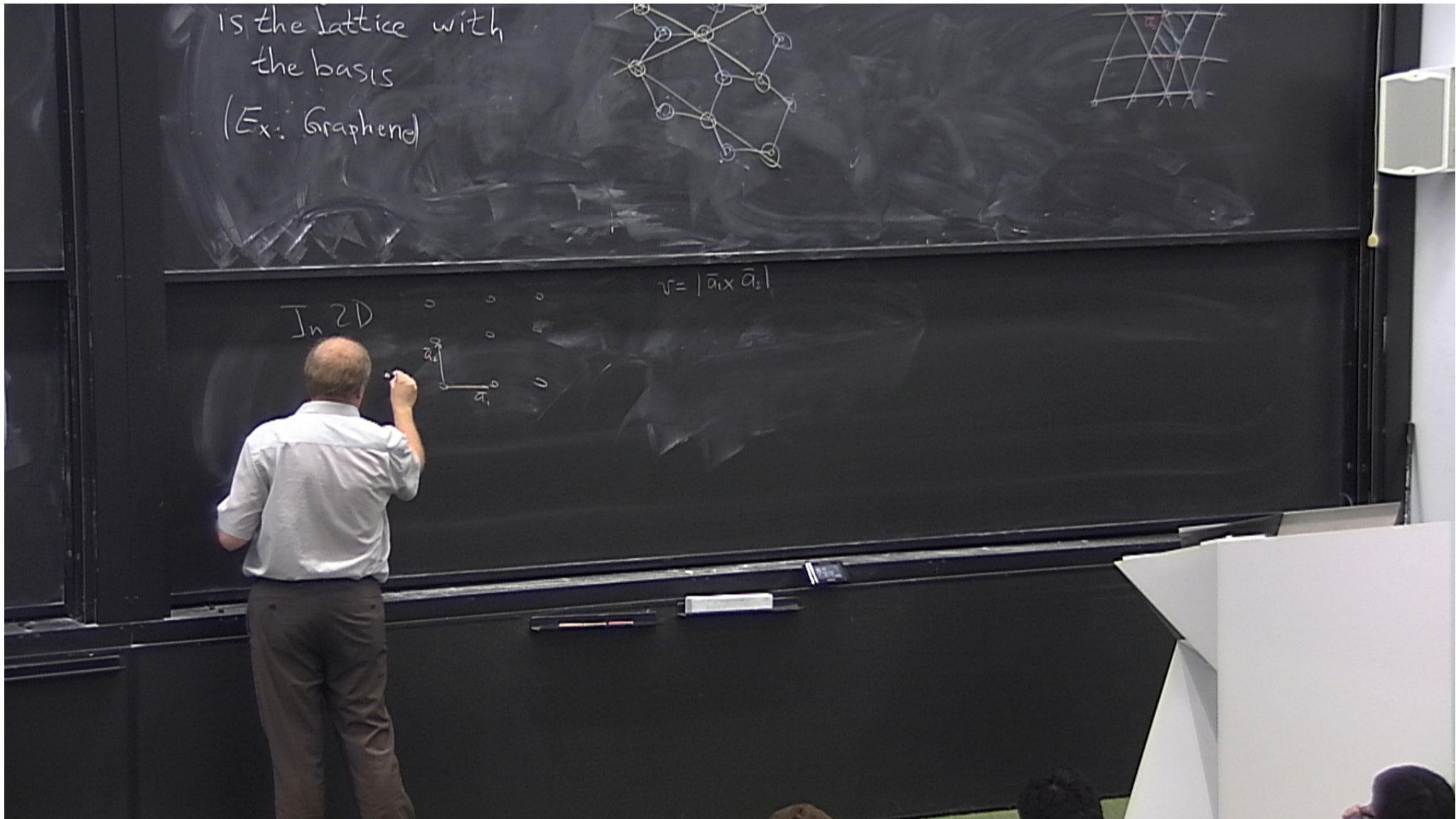


$$|\vec{b}_i \cdot \vec{a}_j| = 2\pi \delta_{ij} \quad \vec{R} = \sum_{\vec{n}} n \cdot \vec{a}_i \quad \vec{K} \cdot \vec{R} = 2\pi \sum_{\vec{n}} n \cdot \vec{k} \Rightarrow \exp\{i \vec{K} \cdot \vec{R}\} = 1$$

(1D) $\vec{a} = a\hat{x}$
RL $\vec{b} = \frac{2\pi}{a}\hat{x}$

3D $v = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$ - volume of the primitive cell

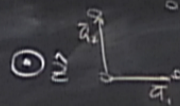
$\vec{b}_1 = \frac{2\pi}{v} \vec{a}_2 \times \vec{a}_3, \vec{b}_2 = \frac{2\pi}{v} \vec{a}_3 \times \vec{a}_1$



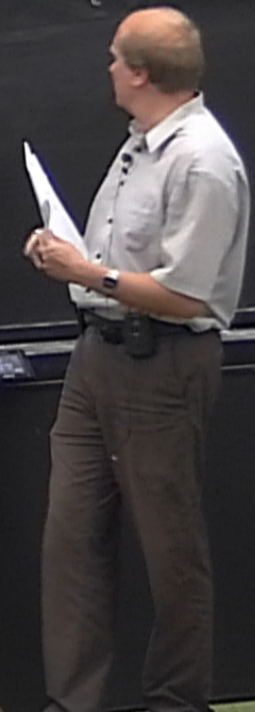
is the lattice with
the basis
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In 2D



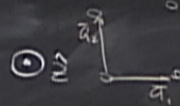
$$r = |\vec{a}_1 \times \vec{a}_2|, \quad \vec{b}_1 = \frac{2\pi}{r} \hat{z} \times \vec{a}_2, \quad \vec{b}_2 = \frac{2\pi}{r} \vec{a}_1 \times \hat{z}$$



is the lattice with
the basis
(Ex: Graphene)

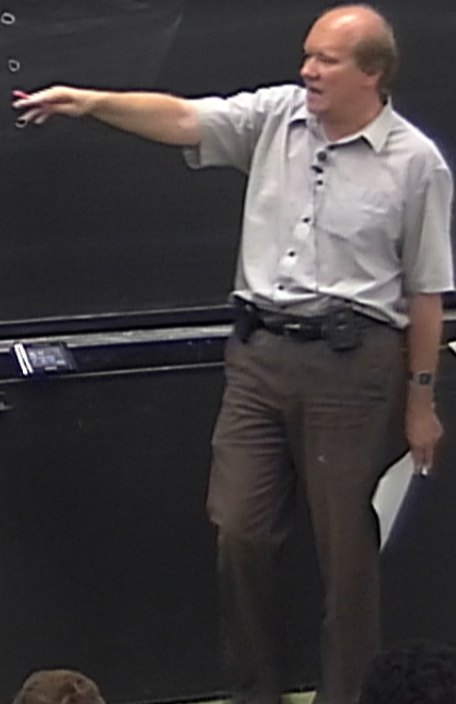


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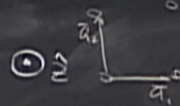
PL



is the lattice with
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In 2D

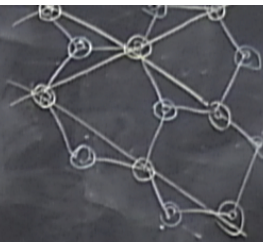


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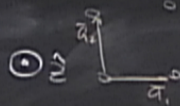


Wigner-Seitz cell for RL is
the first Brillouin zone (1)

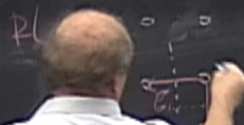
is the lattice with
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(Ex: Graphene)



In 2D

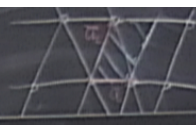


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Wigner-Seitz cell for RL is called
the first Brillouin zone (1BZ)

is the lattice with
the basis



$$|\vec{b}_i \cdot \vec{a}_j| = 2\pi \delta_{ij} \quad \vec{R} = \sum_{i=1}^3 n_i \vec{a}_i \quad \vec{K} \cdot \vec{R} = 2\pi \sum_{i=1}^3 n_i k_i \Rightarrow \exp(i\vec{K} \cdot \vec{R}) = 1$$

(1D)

$$\vec{a} = a\hat{x}$$

$$\vec{b} = \frac{2\pi}{a}\hat{x}$$

RL

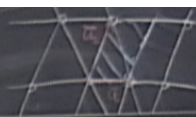
3D $v = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$ - volume of the primitive cell.

$$\vec{b}_1 = \frac{2\pi}{v} \vec{a}_2 \times \vec{a}_3 \quad \vec{b}_2 = \frac{2\pi}{v} \vec{a}_3 \times \vec{a}_1$$

the first Brillouin zone (1BZ)

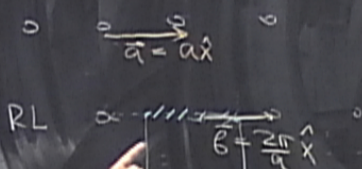
1BZ
for the square lattice

is the lattice with
the basis



$$|\vec{b}_i \cdot \vec{a}_j| = 2\pi \delta_{ij} \quad \vec{R} = \sum_{i=1}^3 n_i \vec{a}_i \quad \vec{k} \cdot \vec{R} = 2\pi \sum_{i=1}^3 n_i k_i \Rightarrow \exp(i\vec{k} \cdot \vec{R}) = 1$$

(1D)



RL

1BZ
for 1D chain

3D $v = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$ - volume of the primitive cell.

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

the first Brillouin zone (1BZ)

1BZ
for the square lattice

IS $\psi(\vec{r})$ satisfies PBC ($L \times L \times L$ box)

$$\psi(\vec{r}) = \sum_{\vec{q}} \psi(\vec{q}) e^{i\vec{q}\vec{r}}$$

$$\psi(\vec{q})$$

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$$\psi(\vec{r}) = \sum_{\vec{q}} \psi(\vec{q}) e^{i\vec{q}\vec{r}}$$

$$\psi(\vec{q}) = \frac{1}{V} \int d\vec{r} \psi(\vec{r}) e^{-i\vec{q}\vec{r}}$$

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$$U(\vec{r}) = U(\vec{r} + \vec{R}) ; \vec{R} \in BL$$

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$$U(\vec{r}) = U(\vec{r} + \vec{R}), \quad \vec{R} \in BL$$

$$U = \sum_{\vec{R}} U$$

IS $\psi(\vec{r})$ satisfies PBC ($L \times L \times L$ box)

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$$\psi(\vec{q}) = \frac{1}{V} \int d\vec{r} \psi(\vec{r}) e^{-i\vec{q}\vec{r}}$$

$$U(\vec{r}) = U(\vec{r} + \vec{R}), \quad \vec{R} \in BL$$

$$U(\vec{r}) = \sum_{\vec{R}} U(\vec{R}) e^{i\vec{R}\vec{r}}$$

IS $\psi(\vec{r})$ satisfies PBC ($L \times L \times L$ box)

$$\psi(\vec{r}) = \sum_{\vec{q}} \psi(\vec{q}) e^{i\vec{q}\vec{r}}$$

$$\psi(\vec{q}) = \frac{1}{V} \int d\vec{r} \psi(\vec{r}) e^{-i\vec{q}\vec{r}}$$

$$U(\vec{r}) = U(\vec{r} + \vec{R}) ; \vec{R} \in BL$$

$$U(\vec{r}) = \sum_{\vec{K}} U(\vec{K}) e^{i\vec{K}\vec{r}}$$

$$U(\vec{K}) = \frac{1}{v} \int d\vec{r} U(\vec{r}) e^{-i\vec{K}\vec{r}}$$

over primitive cell

IS $\psi(\vec{r})$ satisfies PBC ($L \times L \times L$ box)

$$\psi(\vec{r}) = \sum_{\vec{q}} \psi(\vec{q}) e^{i\vec{q}\vec{r}}$$

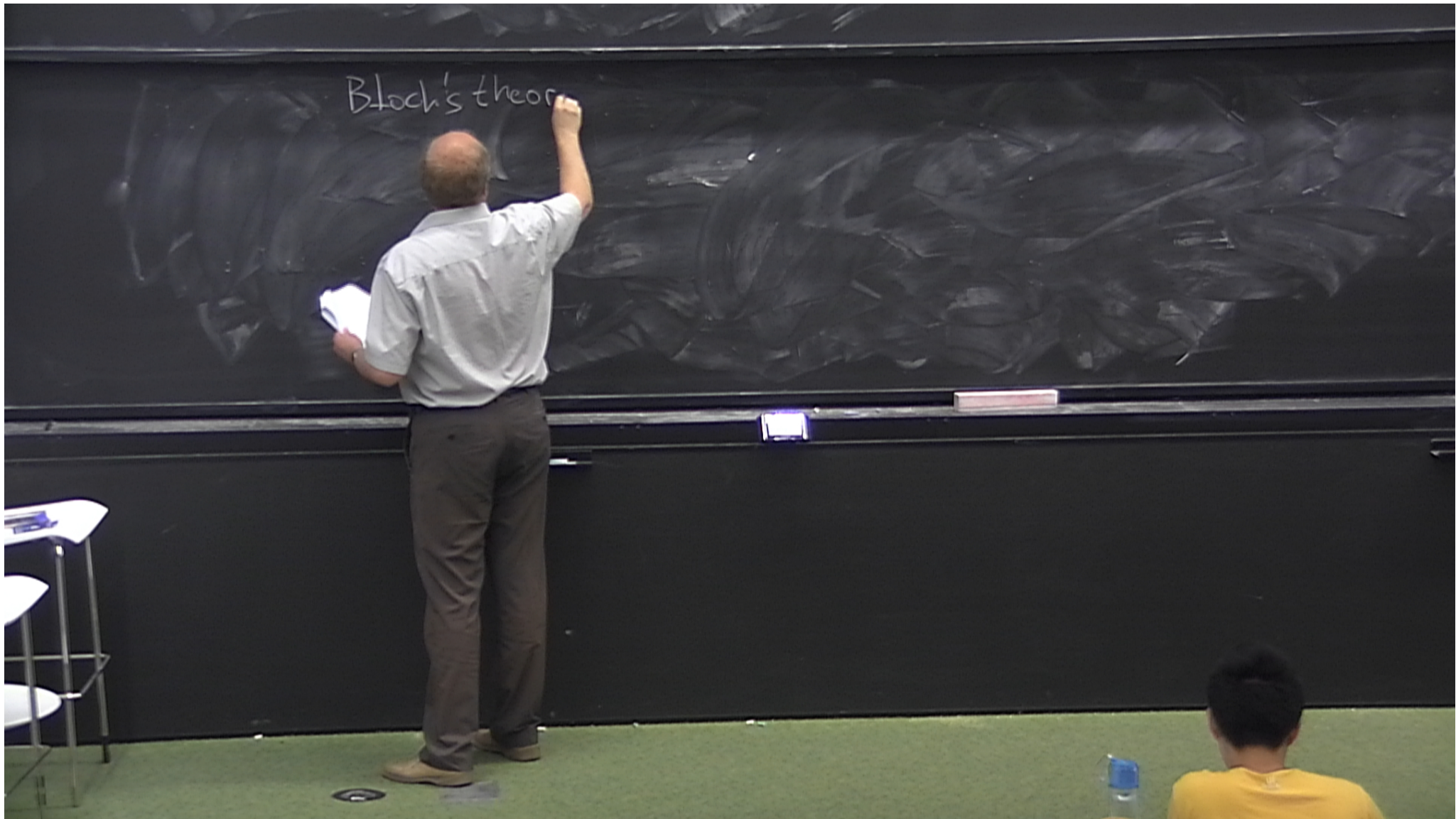
$$\psi(\vec{q}) = \frac{1}{V} \int d\vec{r} \psi(\vec{r}) e^{-i\vec{q}\vec{r}}$$

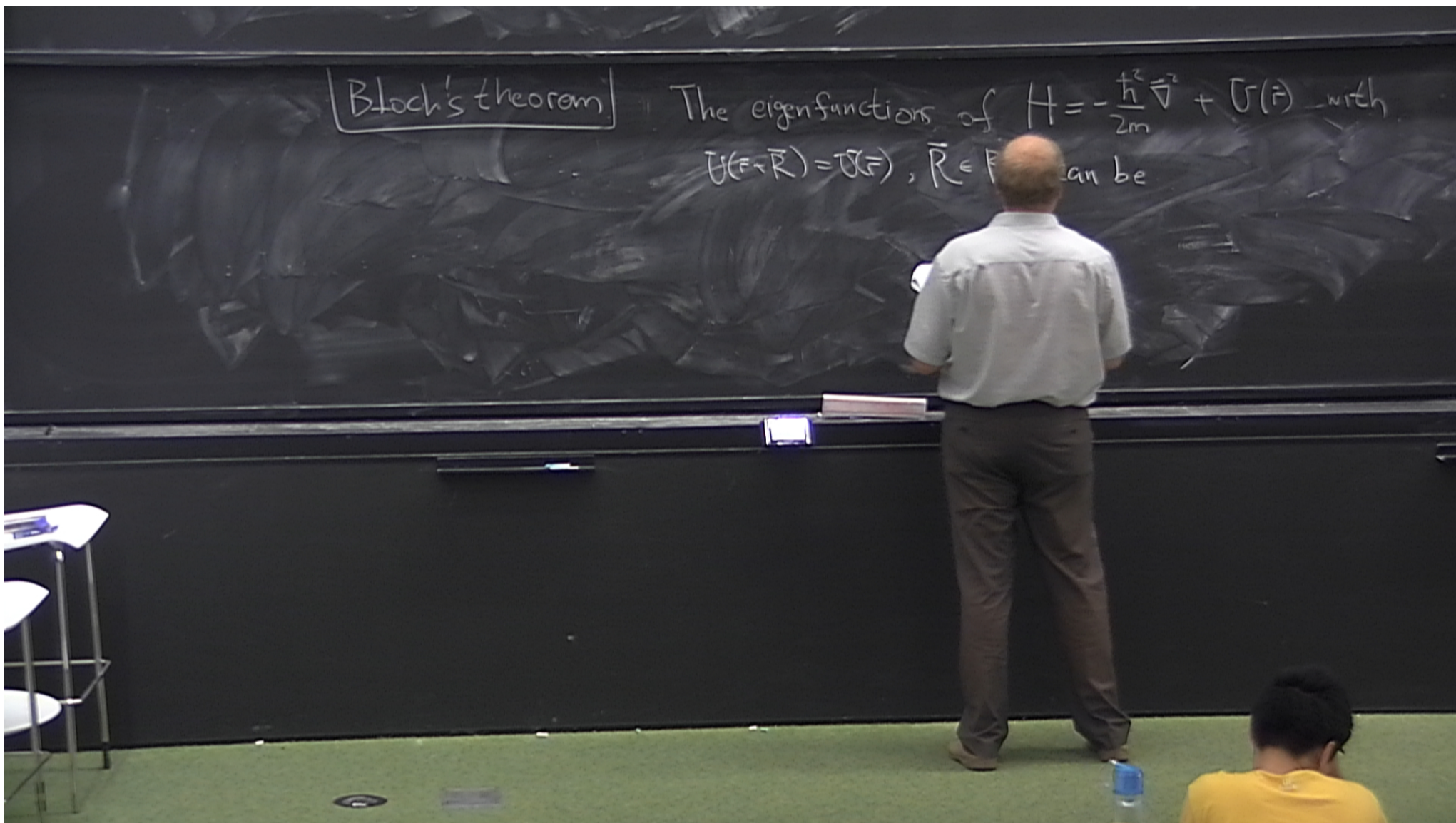
$$U(\vec{r}) = U(\vec{r} + \vec{R}), \quad \vec{R} \in BL_{\vec{R} \neq 0}$$

$$U(\vec{r}) = \sum_{\vec{K}} U(\vec{K}) e^{i\vec{K}\vec{r}}$$

$$U(\vec{K}) = \frac{1}{v} \int d\vec{r} U(\vec{r}) e^{-i\vec{K}\vec{r}}$$

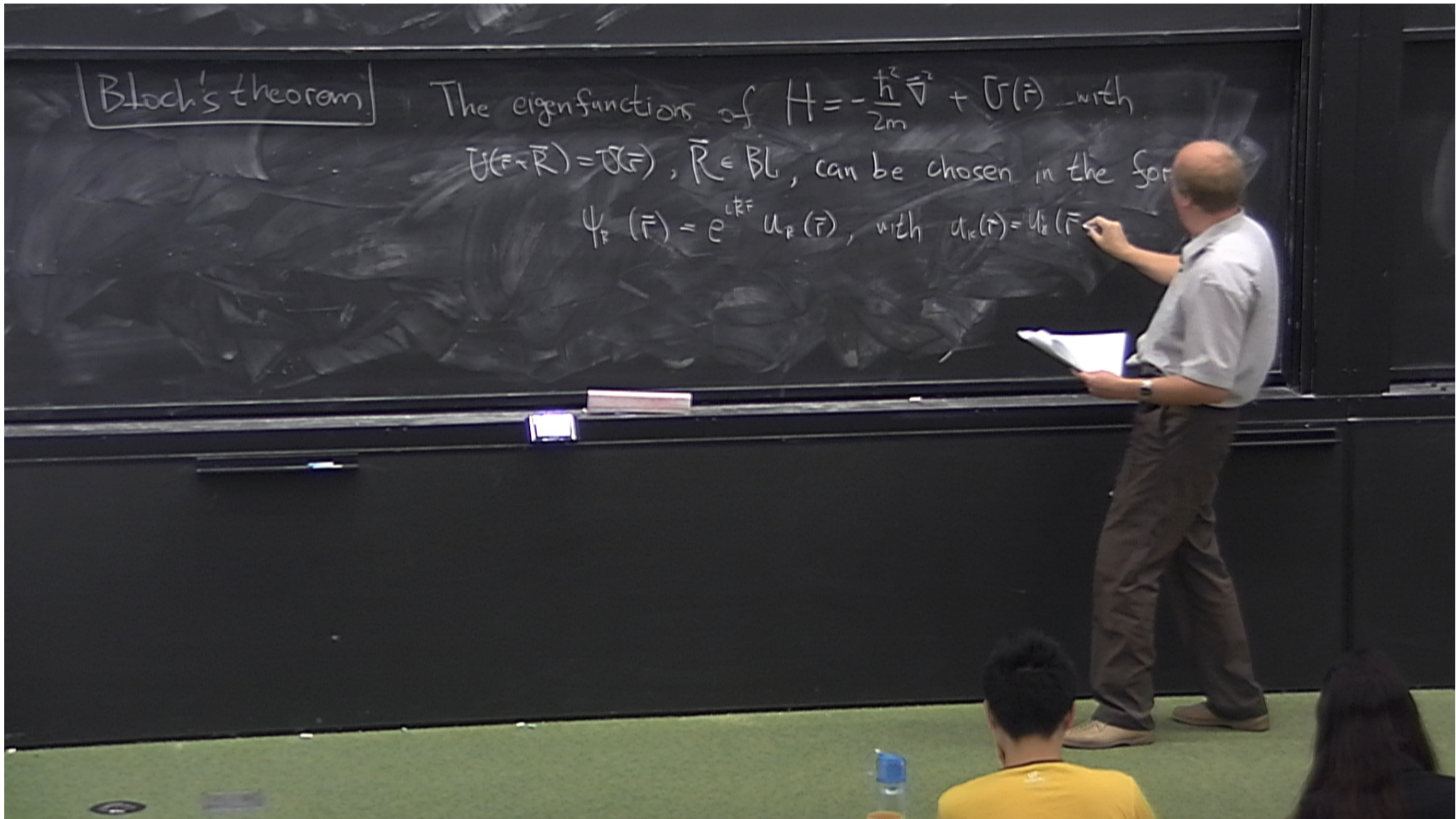
over primitive cell





Bloch's theorem

The eigenfunctions of $H = -\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r})$ with
 $U(\vec{r} + \vec{R}) = U(\vec{r})$, $\vec{R} \in \mathbb{R}^3$ can be

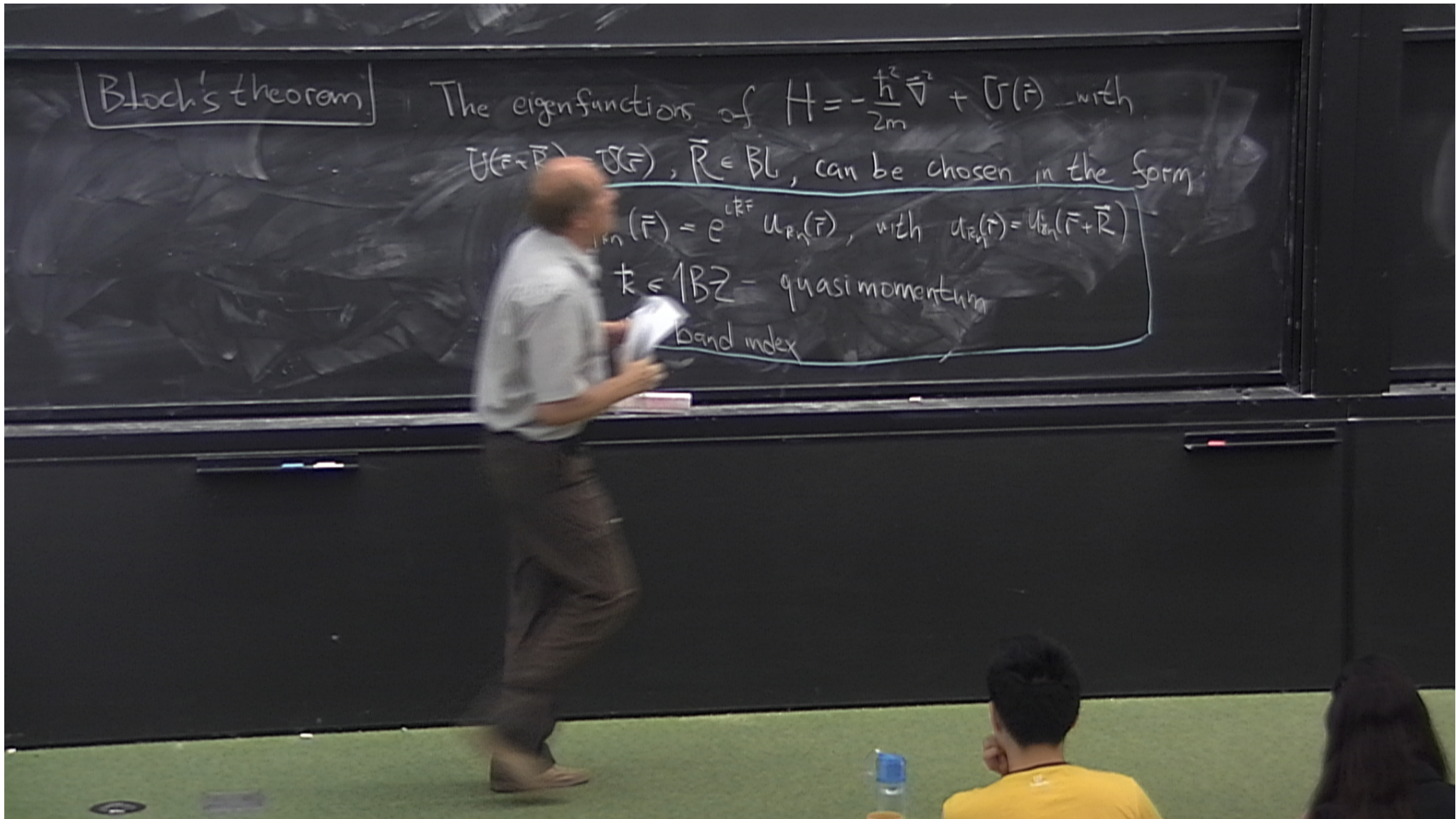


Bloch's theorem

The eigenfunctions of $H = -\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r})$ with

$U(\vec{r} + \vec{R}) = U(\vec{r})$, $\vec{R} \in BL$, can be chosen in the form

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

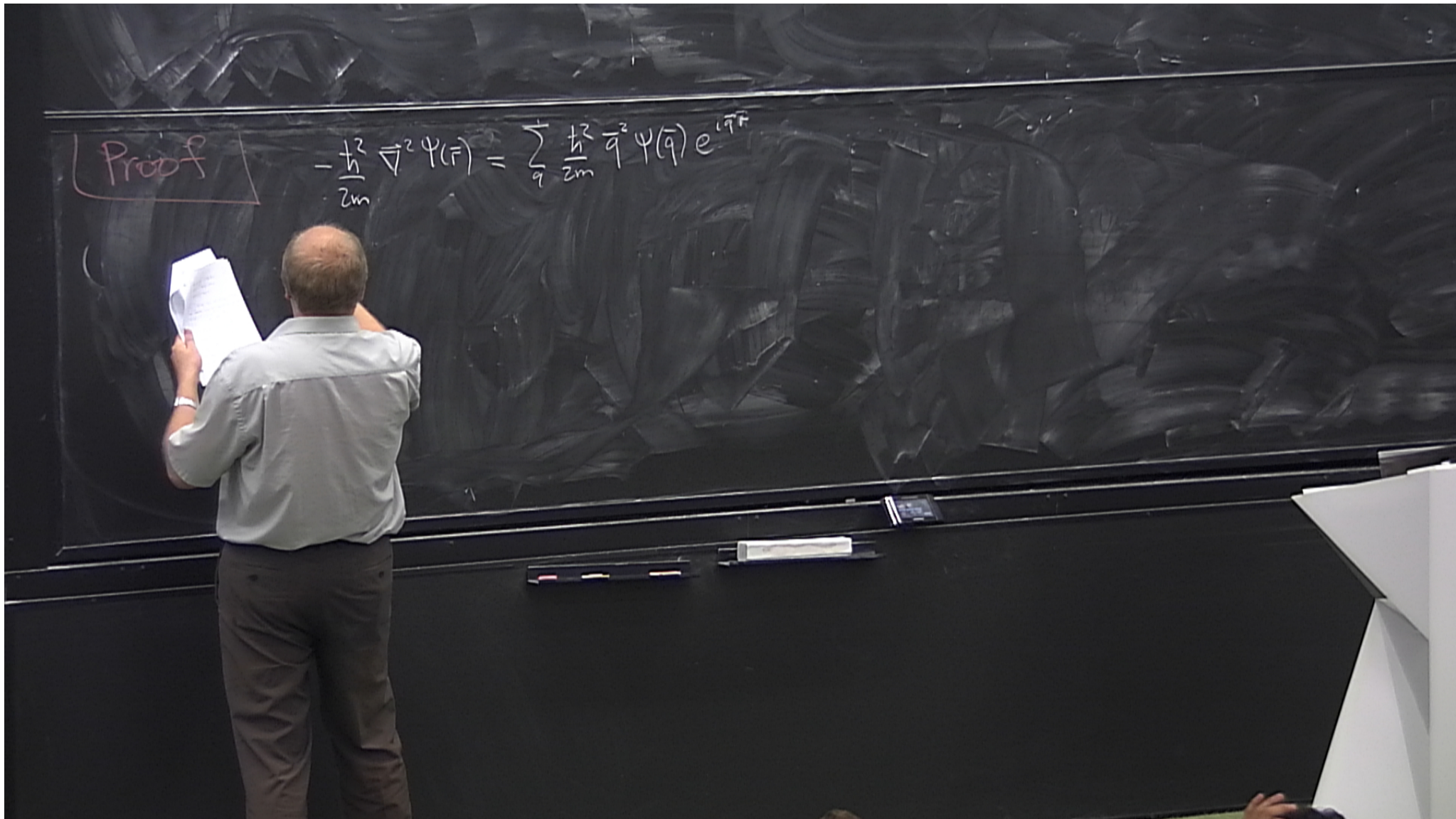


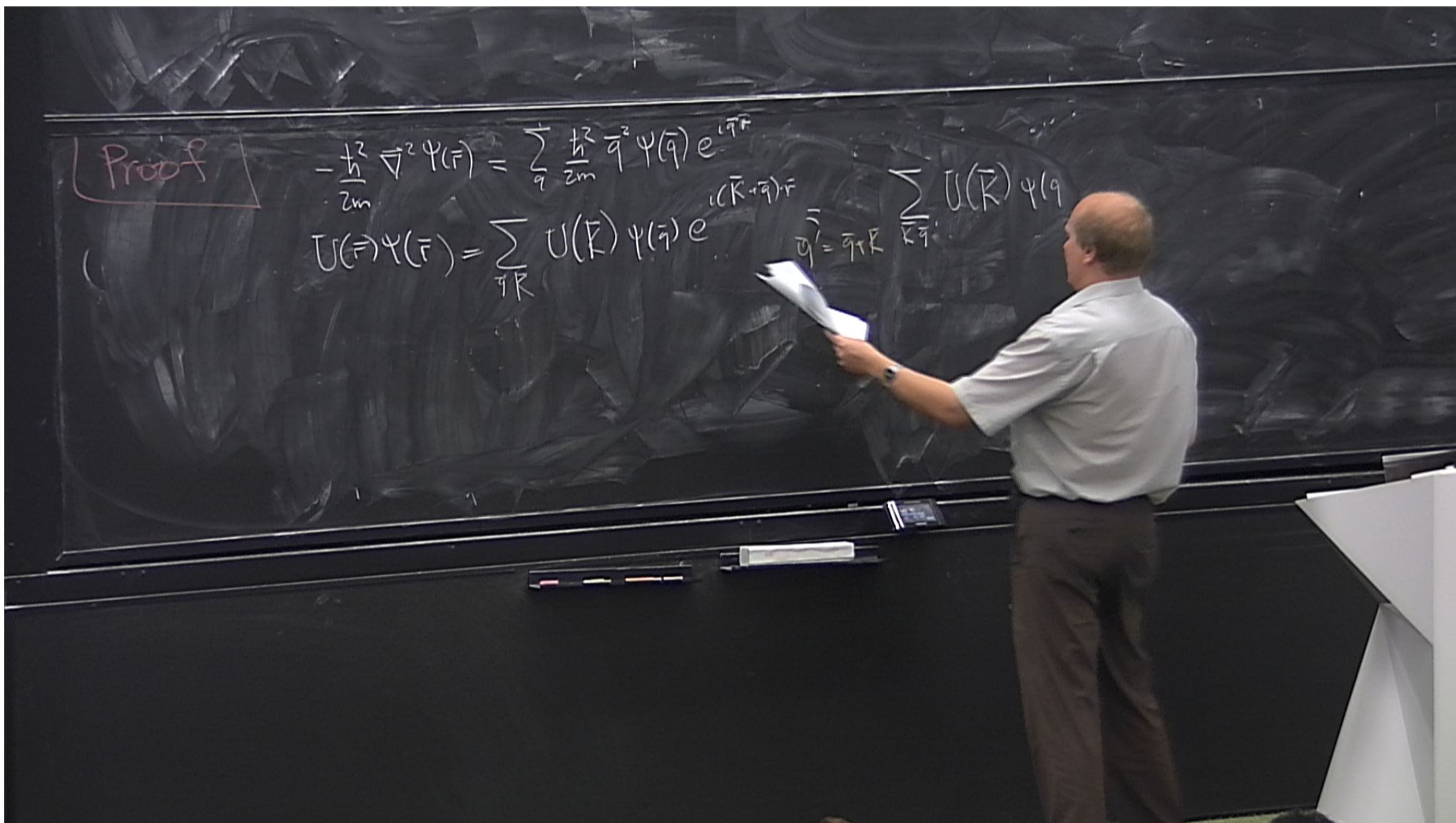
Bloch's theorem

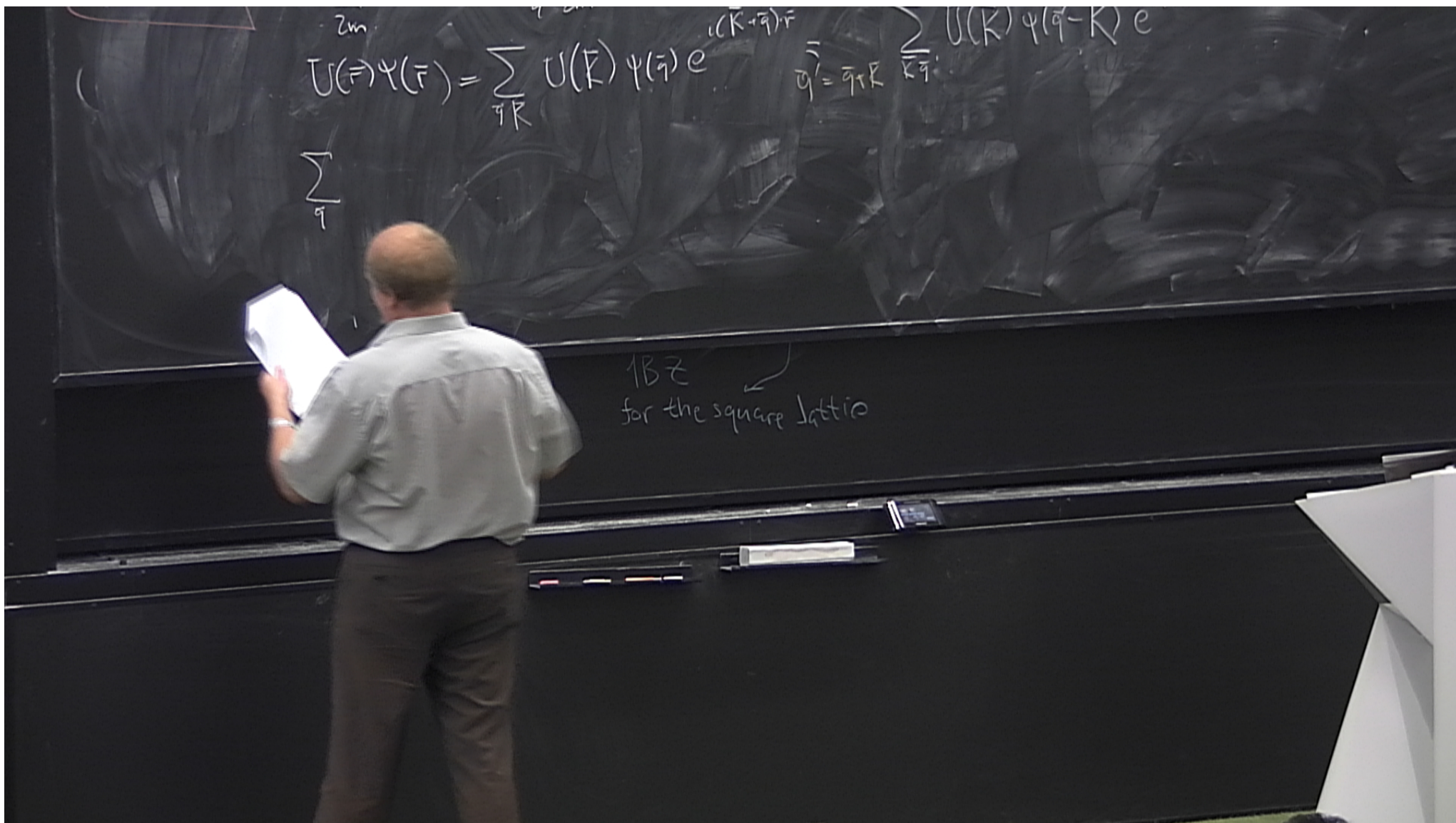
The eigenfunctions of $H = -\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r})$ with $U(\vec{r} + \vec{R}) = U(\vec{r})$, $\vec{R} \in BL$, can be chosen in the form:

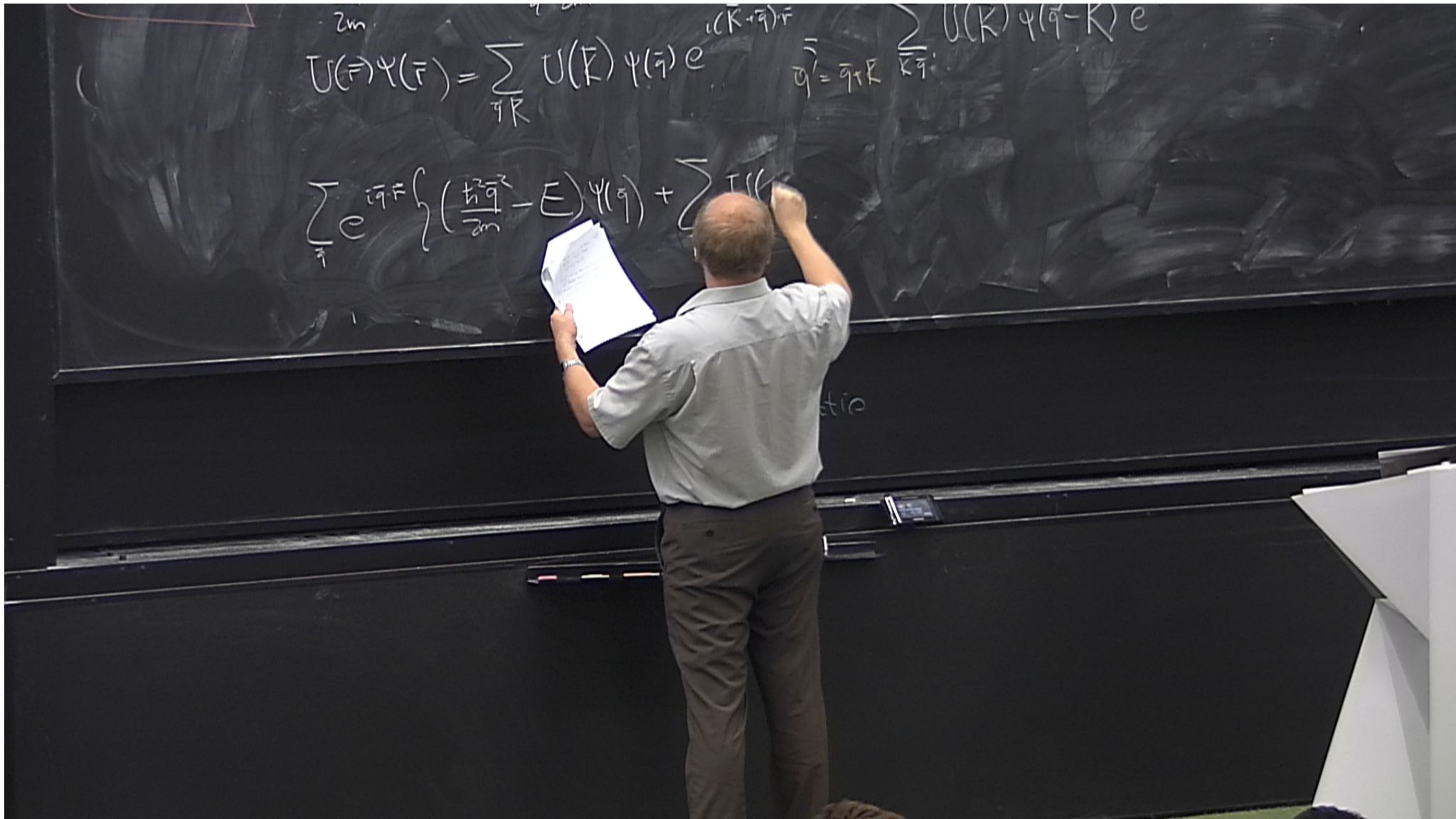
$$\psi_n(\vec{r}) = e^{i\vec{k}\vec{r}} u_{kn}(\vec{r}), \text{ with } u_{kn}(\vec{r}) = u_{kn}(\vec{r} + \vec{R})$$

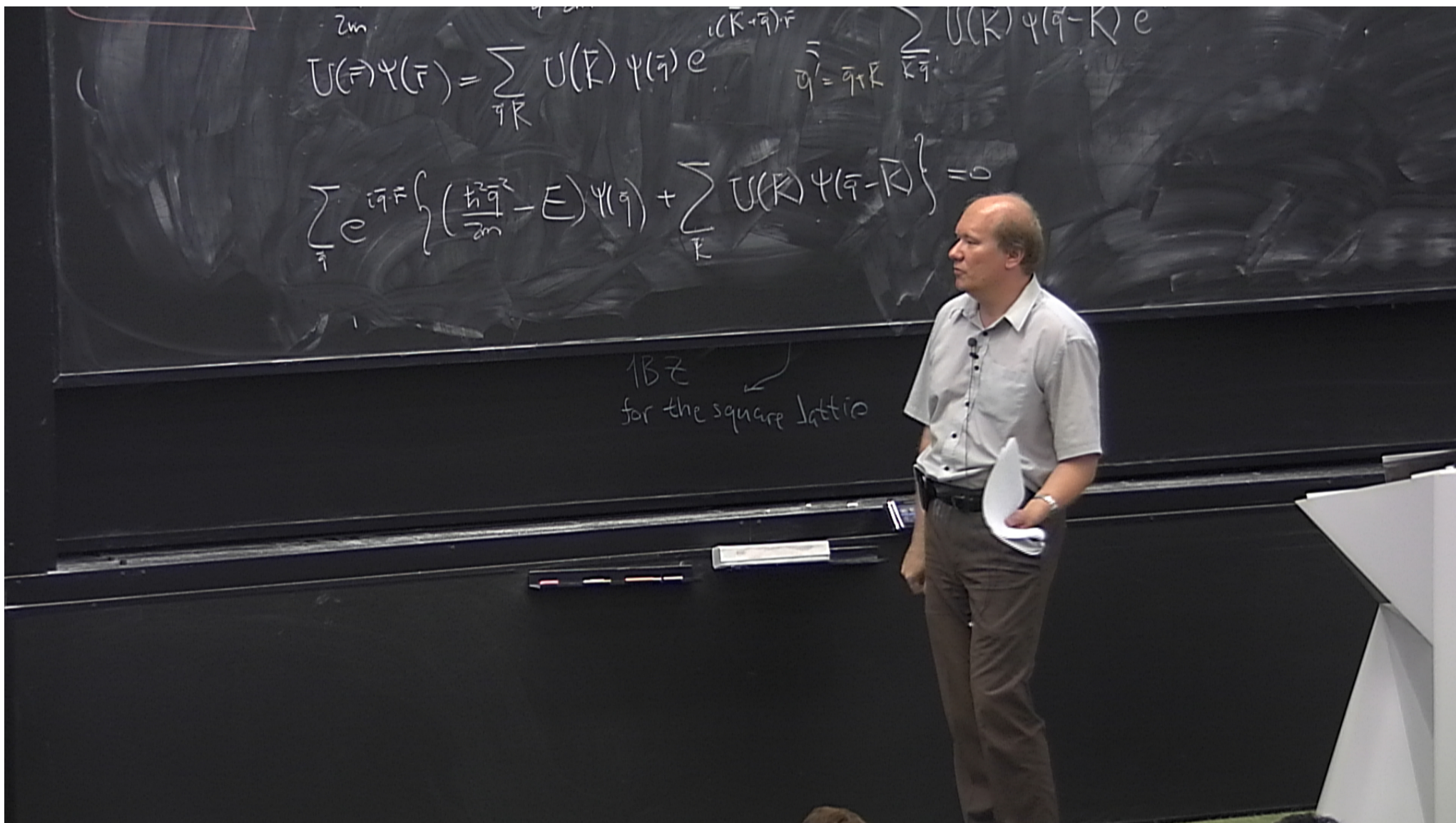
$\vec{k} \in 1BZ$ - quasimomentum
band index

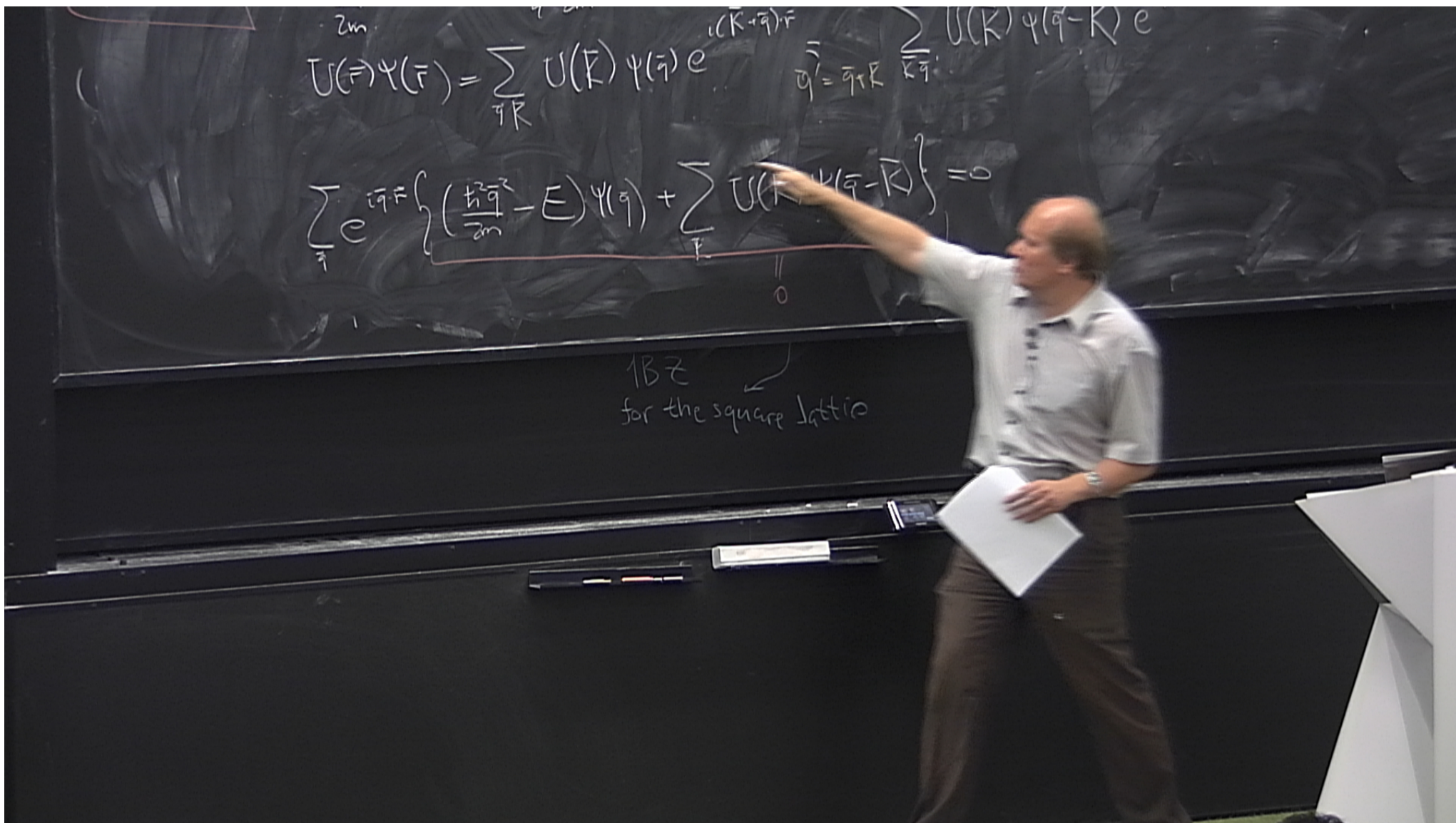












choose $\bar{q} = \bar{k} - \bar{R}$, $\bar{k} \in 1B\mathbb{Z}$ and relabel $\bar{R}' = \bar{R}' - \bar{R}$

$$\left[\frac{\hbar^2}{2m} (\bar{k} - \bar{R}) - E \right] \psi(\bar{k} - \bar{R}) + \sum_{\bar{R}'} U(\bar{R}' - \bar{R}) \psi(\bar{k} - \bar{R}') = 0$$

choose $\bar{q} = \frac{1}{2} - \bar{K}$, $\frac{1}{2} \in 1B\mathbb{Z}$ and relabel $\bar{K}' = \bar{K}' - \bar{K}$

$$\left[\frac{\hbar^2}{2m} (\frac{1}{2} - \bar{K})^2 - E \right] \psi(\frac{1}{2} - \bar{K}) + \sum_{\bar{K}'} U(\bar{K}' - \bar{K}) \psi(\frac{1}{2} - \bar{K}') = 0$$

choose $\bar{q} = \bar{k} - \bar{K}$, $\bar{k} \in 1B\mathbb{Z}$ and relabel $\bar{K}' = \bar{K}' - \bar{K}$

$$\left[\frac{\hbar^2}{2m} (\bar{k} - \bar{K})^2 - E \right] \psi(\bar{k} - \bar{K}) + \sum_{\bar{K}'} U(\bar{K}' - \bar{K}) \psi(\bar{k} - \bar{K}') = 0$$

If $\bar{k} \in 1B\mathbb{Z}$ is fixed then the system determines $\psi(\bar{k})$

choose $\vec{q} = \vec{k} - \vec{K}$, $\vec{k} \in 1BZ$ and relabel $\vec{K}' = \vec{K}' - \vec{K}$

$$\left[\frac{\hbar^2}{2m} (\vec{k} - \vec{K})^2 - E \right] \psi(\vec{k} - \vec{K}) + \sum_{\vec{K}'} U(\vec{K}' - \vec{K}) \psi(\vec{k} - \vec{K}') = 0$$

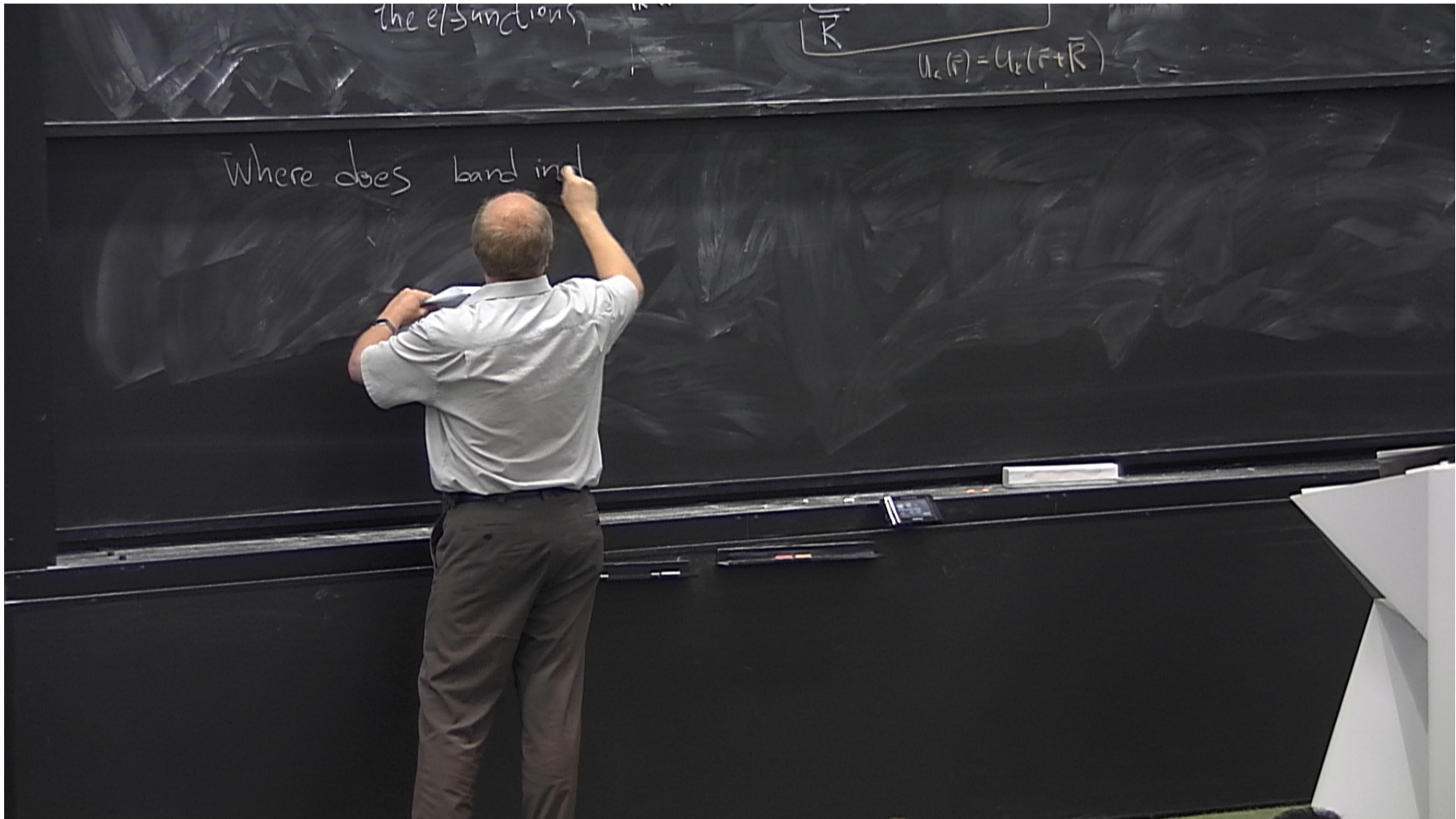
If $\vec{k} \in 1BZ$ is fixed then the system determines $\psi(\vec{k}), \psi(\vec{k} - \vec{K}'), \psi(\vec{k} - \vec{K}'')$

choose $\vec{q} = \vec{k} - \vec{K}$, $\vec{k} \in 1BZ$ and relabel $\vec{K}' = \vec{K} - \vec{K}$

$$\left[\frac{\hbar^2}{2m} (\vec{k} - \vec{K})^2 - E \right] \psi(\vec{k} - \vec{K}) + \sum_{\vec{K}'} U(\vec{K}' - \vec{K}) \psi(\vec{k} - \vec{K}') = 0$$

If $\vec{k} \in 1BZ$ is fixed then the system determines $\psi(\vec{k}), \psi(\vec{k} - \vec{K}'), \psi(\vec{k} - \vec{K}'')$

the el/s functions $\psi_{\vec{K}}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} \psi(\vec{k} - \vec{K}) e^{-i\vec{K} \cdot \vec{r}}$

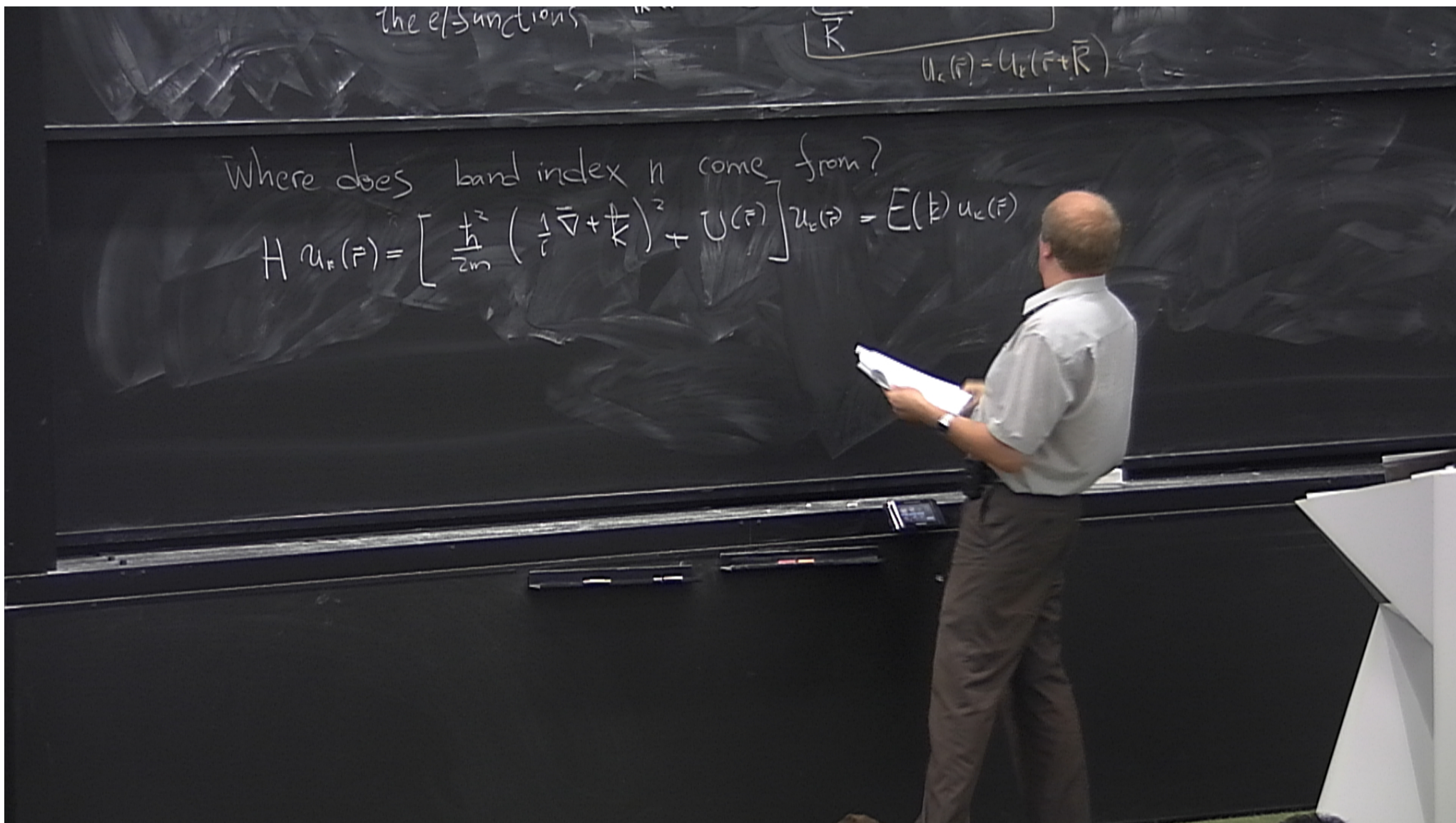


the e/s functions

$\bar{R}$

$$U_c(\vec{r}) = U_c(\vec{r} + \bar{R})$$

Where does band index n come from?



the e/s functions

$\vec{R}$

$$u_k(\vec{r}) = u_k(\vec{r} + \vec{R})$$

Where does band index n come from?

$$H u_k(\vec{r}) = \left[\frac{\hbar^2}{2m} \left(\frac{1}{i} \vec{\nabla} + \vec{k} \right)^2 + U(\vec{r}) \right] u_k(\vec{r}) = E(k) u_k(\vec{r}), \quad u_k(\vec{r}) = u_k(\vec{r} + \vec{R})$$

$\Downarrow$

Sch eq for $u_k(\vec{r})$ obey on a primitive cell

the e/s functions

$\vec{R}$

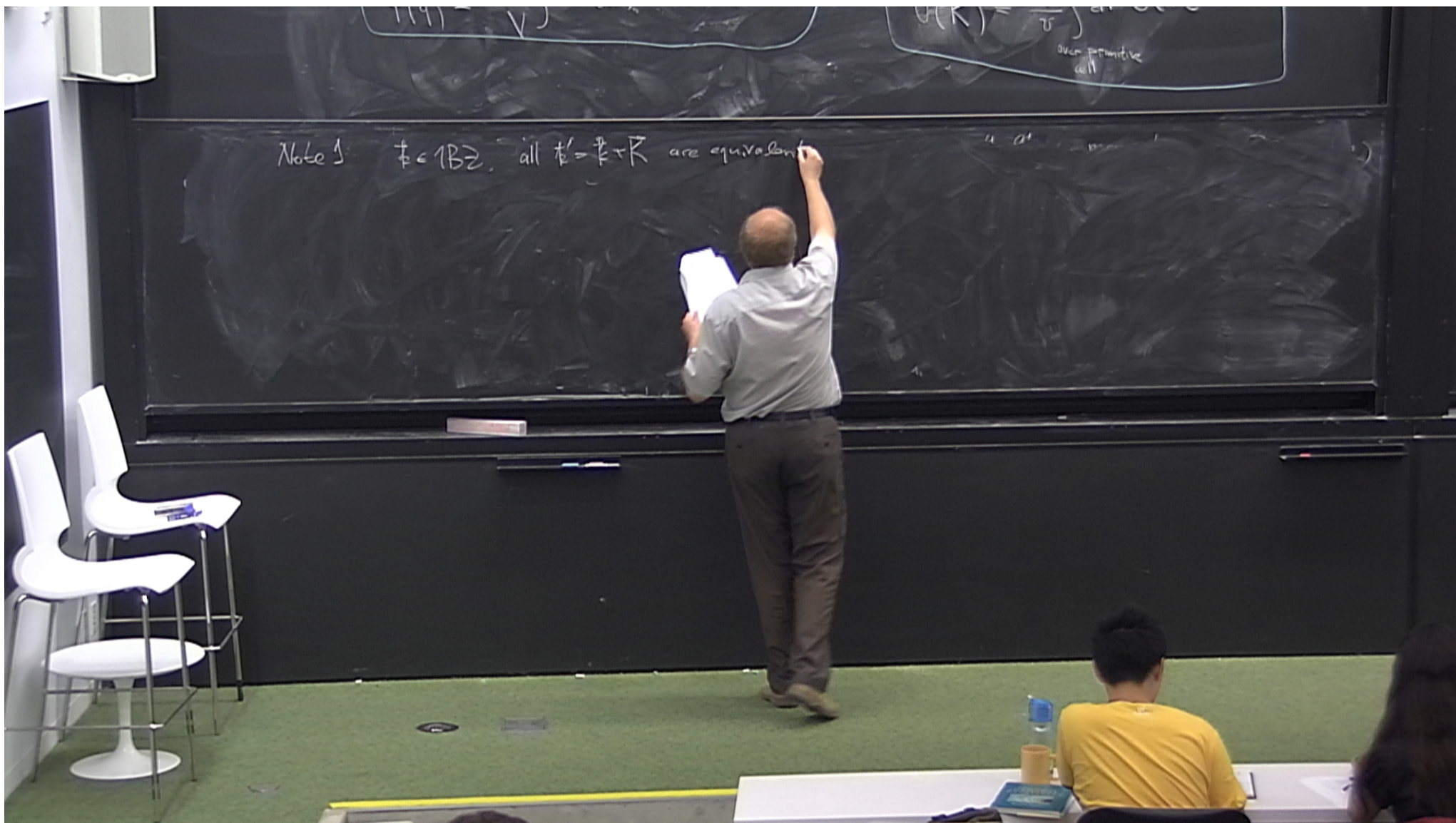
$$u_k(\vec{r}) = u_k(\vec{r} + \vec{R})$$

Where does band index n come from?

$$H u_k(\vec{r}) = \left[\frac{\hbar^2}{2m} \left(\frac{1}{i} \vec{\nabla} + \vec{k} \right)^2 + U(\vec{r}) \right] u_k(\vec{r}) = E_k(\vec{k}) u_k(\vec{r}), \quad u_k(\vec{r}) = u_k(\vec{r} + \vec{R})$$

$\Downarrow$

Sch eq for $u_k(\vec{r})$ obeying P a primitive cell $\Rightarrow$ additional index



Note 1: $k \in \mathbb{B}\mathbb{Z}$, all $k' = k + R$ are equivalent $\Rightarrow \psi_{nE}(z) = \psi_{nE+R}(z)$
 $E_{nE} = E_{nE+R}$
 $E_n(k)$

Note 1. $k \in \mathbb{BZ}$, all $k' = k + K$ are equivalent $\Rightarrow \psi_{nE}(\vec{r}) = \psi_{nE+K}(\vec{r})$

Note 1. k should not be confused with $k \nabla$

$\psi_{kn}(\vec{r})$ are not eigenfunctions

$$E_{nE} = E_{nE+K}$$

$$E_n(k)$$