Title: 14/15 PSI - Condensed Matter-Lecture 8

Date: Nov 19, 2014 10:45 AM

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Abstract:

ELECTRONS IN PERIODIC POTENTIAL

$$H = \frac{p^2}{2m} + U(\vec{r}), \quad U(\vec{r}+\vec{R}) = U(\vec{r})$$

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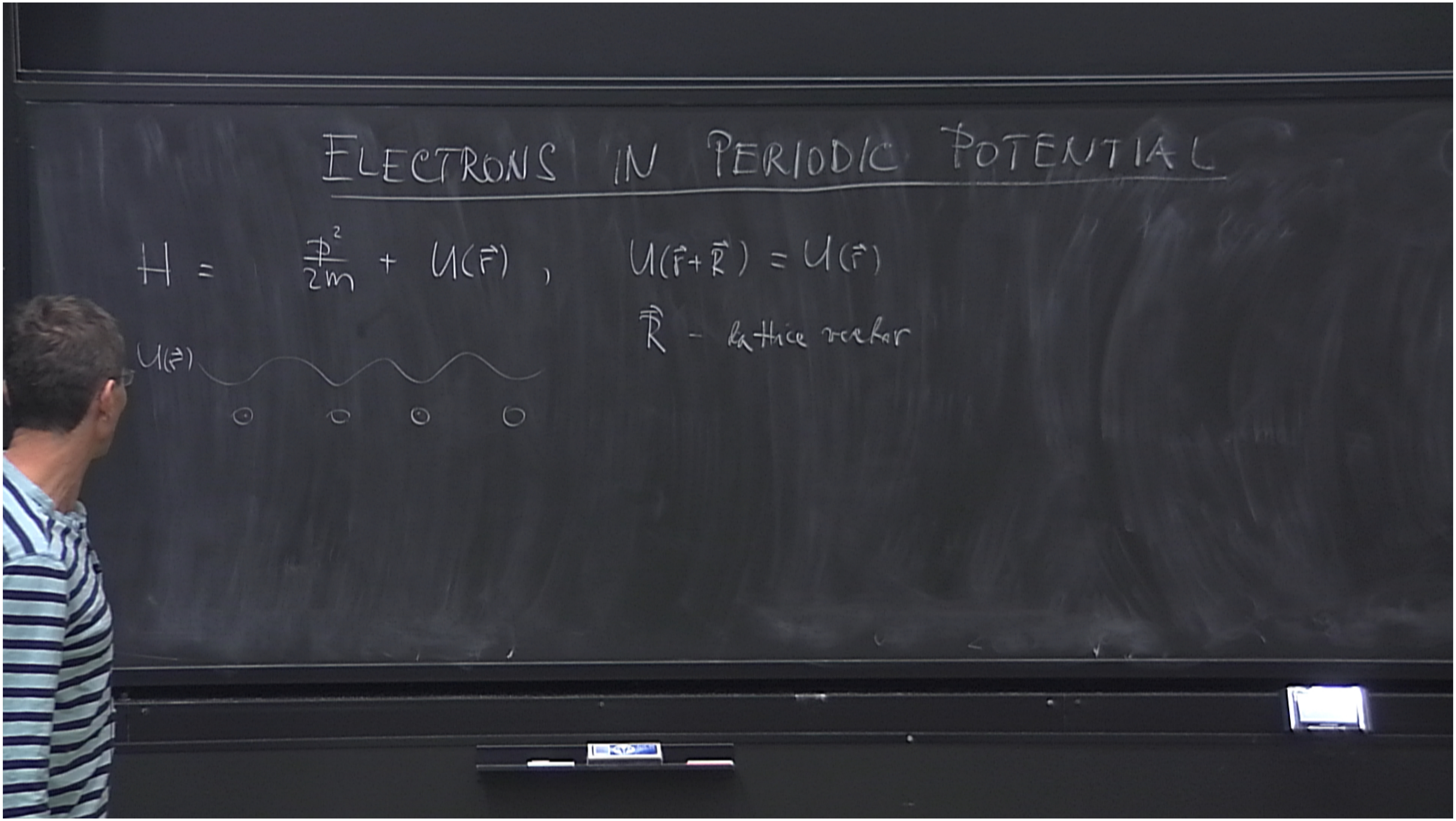
ELECTRONS IN PERIODIC POTENTIAL
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$\vec{R}$ - lattice vector
$U(\vec{r})$

ELECTRONS IN PERIODIC POTENTIAL

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Bloch theorem: The eigenstates of H can be chosen to have the form $\psi_{nk}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{nk}(\vec{r})$ with $u_{nk}(\vec{r}+\vec{R}) = u_{nk}(\vec{r})$.

ELECTRONS IN PERIODIC POTENTIAL

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Alternative statement:

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

Alternative statement:

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

PROOF:

Define operator $T_{\vec{R}}$

$$T_{\vec{R}}\, f(\vec{r}) = f(\vec{r} + \vec{R})$$

Alternative statement:

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

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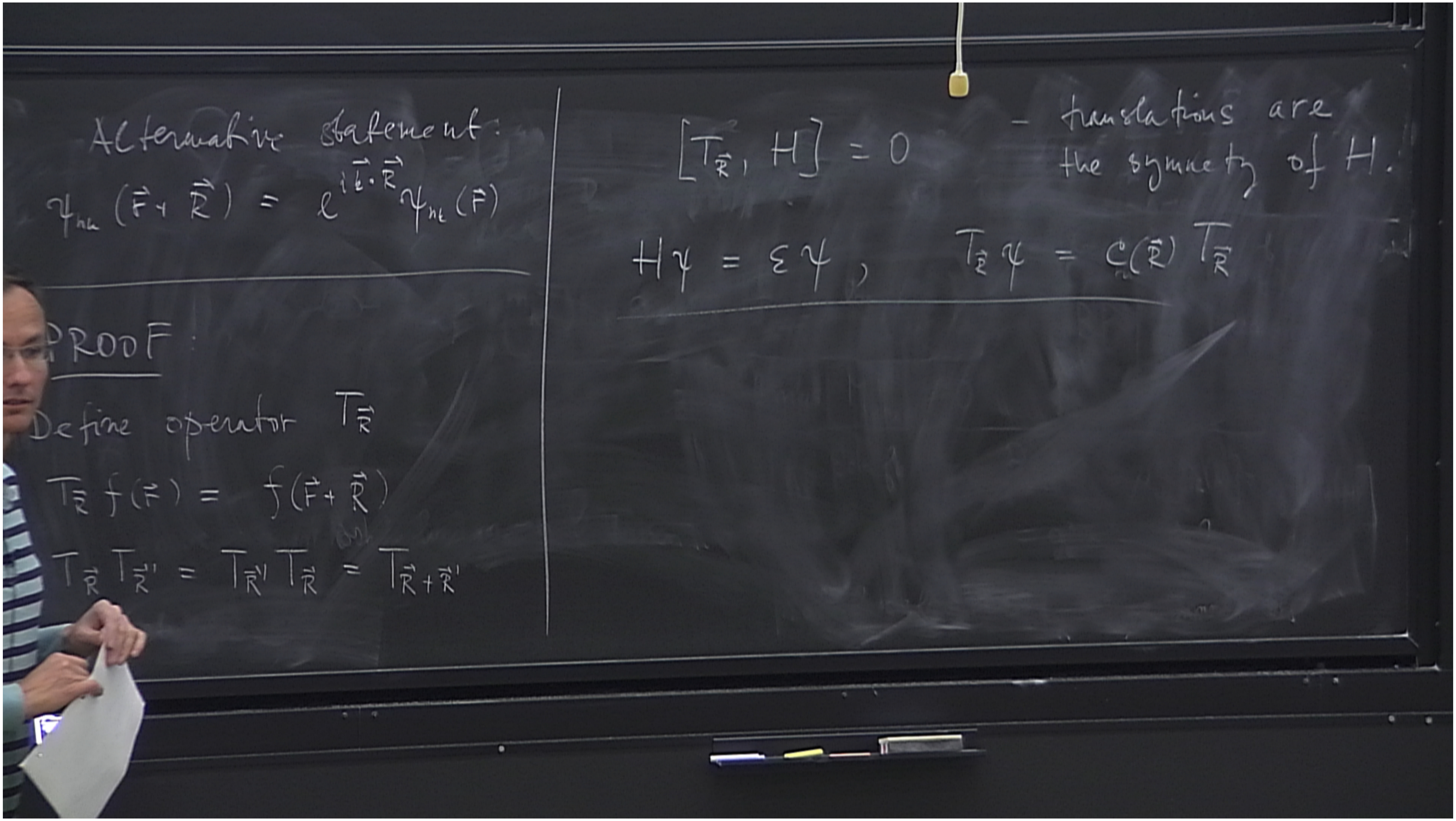
$$[T_{\vec{R}}, H] = 0$$

– translations are the symmetry of H.



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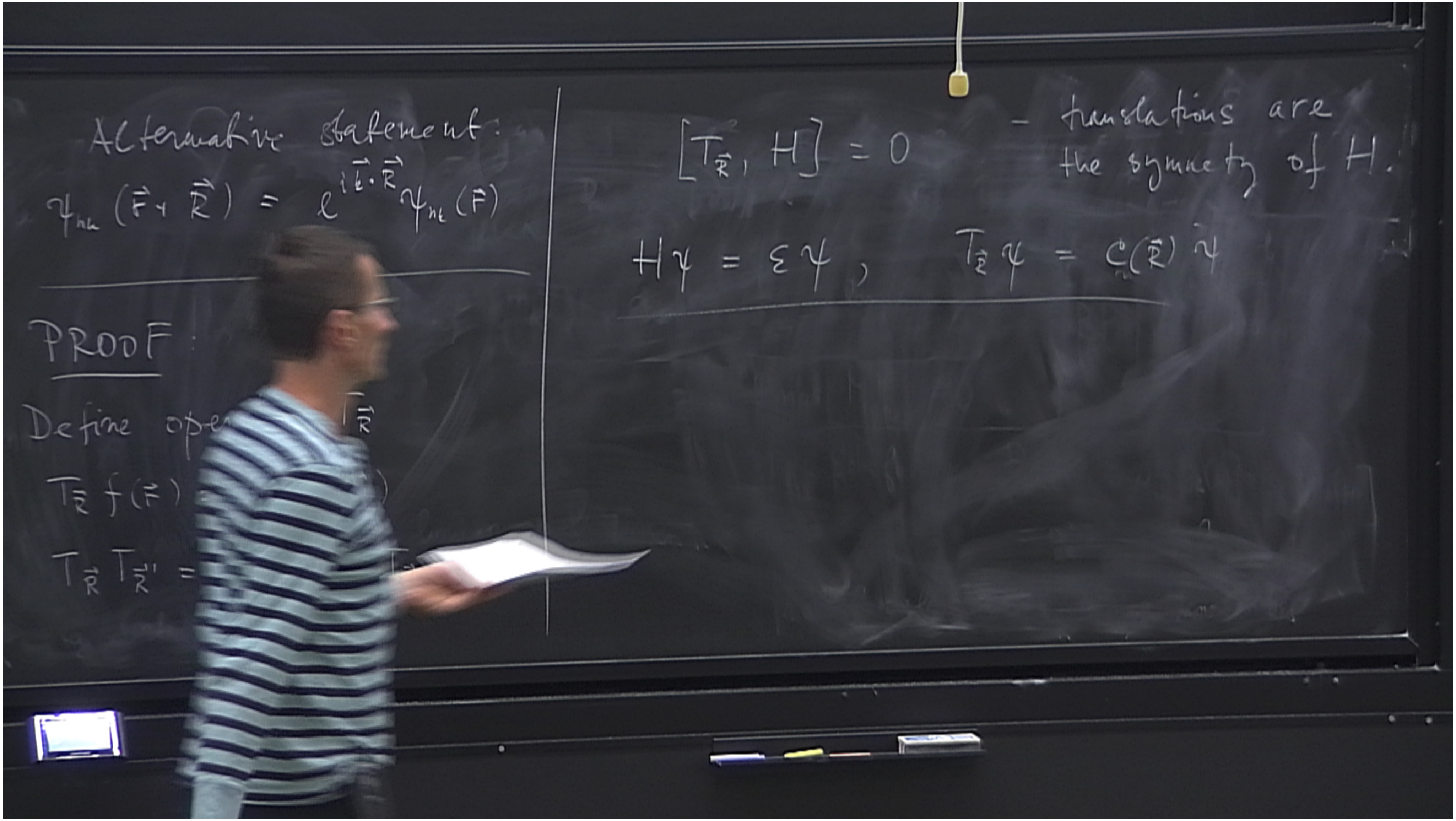
$[T_{\vec{R}}, H] = 0$ – translations are the symmetry of H.
$H\psi = \varepsilon\psi$, $T_{\vec{R}}\psi = c(\vec{R})\, T_{\vec{R}}$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$$H\psi = \varepsilon\psi, \quad T_{\vec{R}}\psi = c(\vec{R})\psi$$

$$T_{R} T_{R'}\psi = T_{R+R'}\psi = c(\vec{R}+\vec{R}')\psi$$

$$\Rightarrow c(\vec{R}+\vec{R}') = c(\vec{R})\,c(\vec{R}')$$

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$$[T_{\vec{R}}, H] = 0$$ – translations are the symmetry of H.

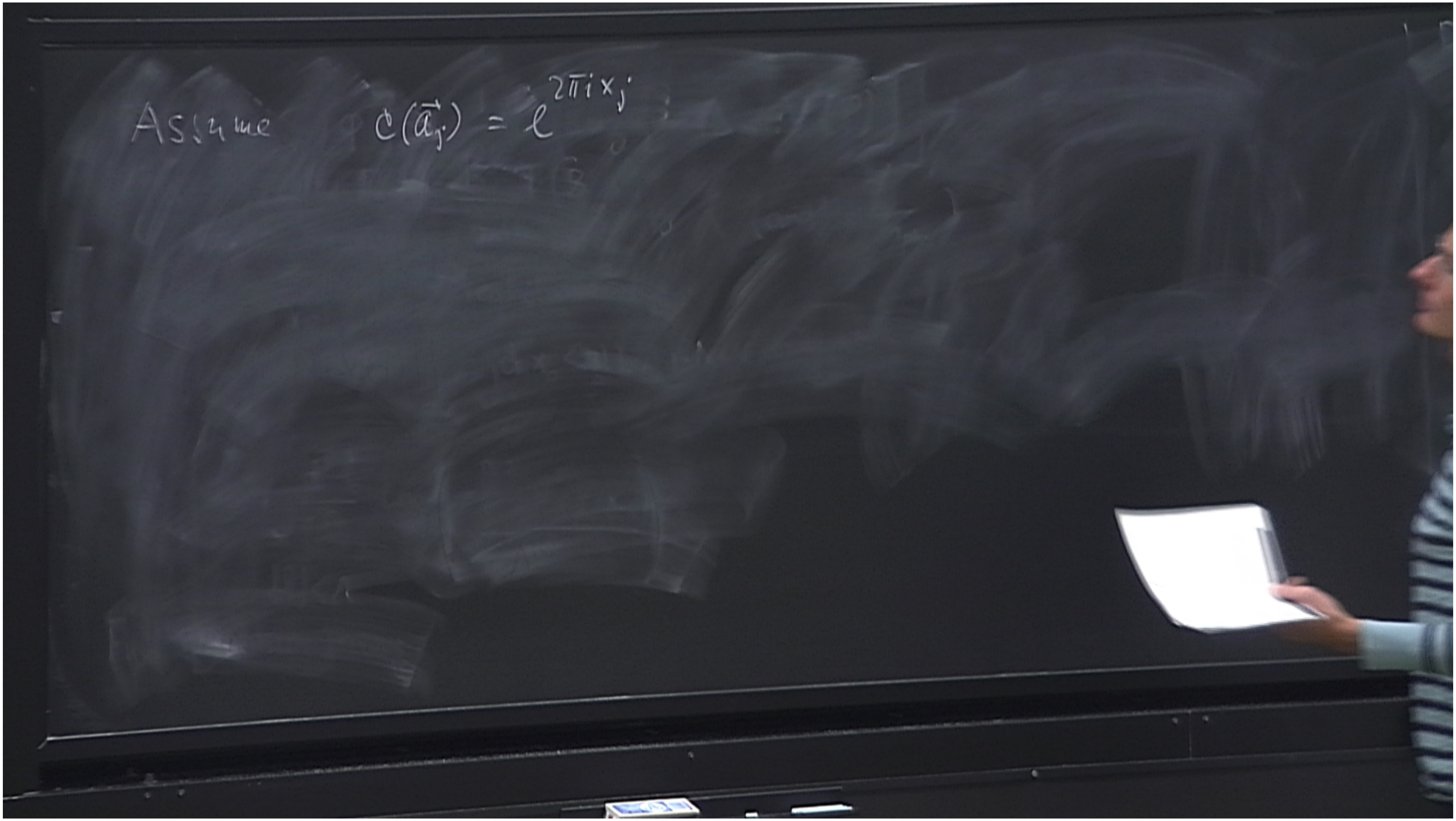
$$H\psi = \varepsilon\psi, \quad T_{\vec{R}}\psi = c(\vec{R})\psi$$

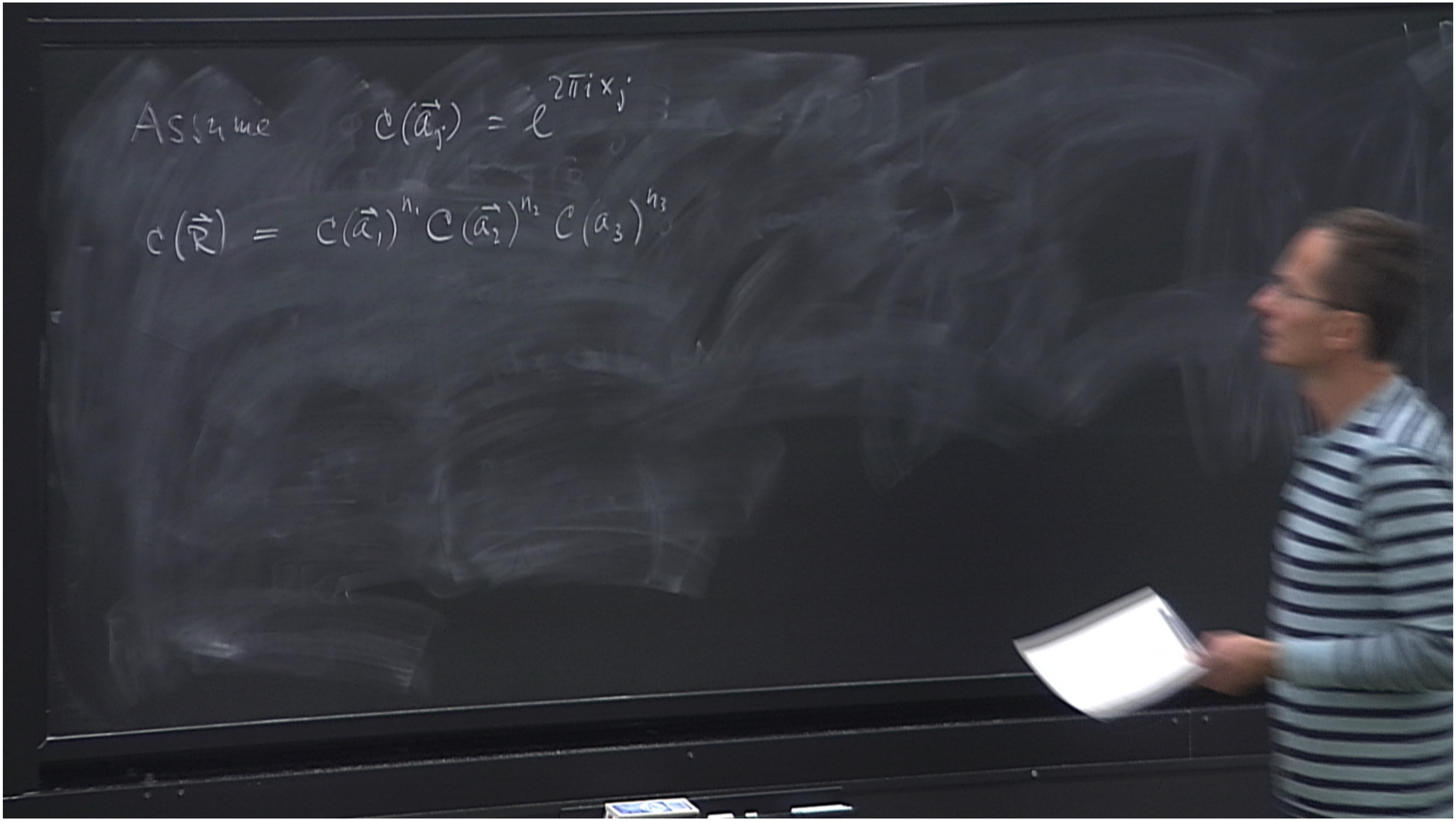
$$T_{\vec{R}} T_{\vec{R}'}\psi = T_{\vec{R}+\vec{R}'}\psi = c(\vec{R}+\vec{R}')\psi$$

$$\Rightarrow c(\vec{R}+\vec{R}') = c(\vec{R})c(\vec{R}')$$

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

$\vec{a}_j$ – primitive latt. vectors, $n_j \in \mathbb{Z}$


Assume $c(\vec{a}_j) = e^{2\pi i x_j}$


Assume $c(\vec{a}_j) = e^{2\pi i x_j}$
$c(\vec{R}) = c(\vec{a}_1)^{n_1} c(\vec{a}_2)^{n_2} c(a_3)^{n_3}$

Assume $c(\vec{a}_j) = e^{2\pi i x_j}$

$$c(\vec{R}) = c(\vec{a}_1)^{n_1} c(\vec{a}_2)^{n_2} c(\vec{a}_3)^{n_3}$$

$\Rightarrow c(\vec{R}) = e^{i\vec{k}\cdot\vec{R}}$ with $\vec{k} = x_1\vec{b}_1 + x_2\vec{b}_2 + x_3\vec{b}_3$

$\vec{b}_j$ - rec latt. primitive vectors, $\vec{b}_i \cdot \vec{a}_j = 2\pi\delta_{ij}$

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Assume $C(\vec{a}_j) = e^{2\pi i x_j}$

$$C(\vec{R}) = C(\vec{a}_1)^{n_1} C(\vec{a}_2)^{n_2} C(\vec{a}_3)^{n_3}$$

$\Rightarrow \underline{C(\vec{R}) = e^{i\vec{k}\cdot\vec{R}}}$ with $\vec{k} = x_1 \vec{b}_1 + x_2 \vec{b}_2 + x_3 \vec{b}_3$

$\vec{b}_j$ - rec latt. primitive vectors, $\vec{b}_i \cdot \vec{a}_j = 2\pi\,\delta_{ij}$

$$T_R\,\psi(\vec{r}) = \underline{\psi(\vec{r}+\vec{R})} = C(\vec{R})\,\psi(\vec{r}) = \underline{e^{i\vec{k}\cdot\vec{R}}\,\psi(\vec{r})},$$

Assume $c(\vec{a}_j) = e^{2\pi i x_j}$

$$c(\vec{R}) = c(\vec{a}_1)^{n_1} c(\vec{a}_2)^{n_2} c(\vec{a}_3)^{n_3}$$

$$\Rightarrow \underline{c(\vec{R}) = e^{i\vec{k}\cdot\vec{R}}} \quad \text{with} \quad \vec{k} = x_1\vec{b}_1 + x_2\vec{b}_2 + x_3\vec{b}_3$$

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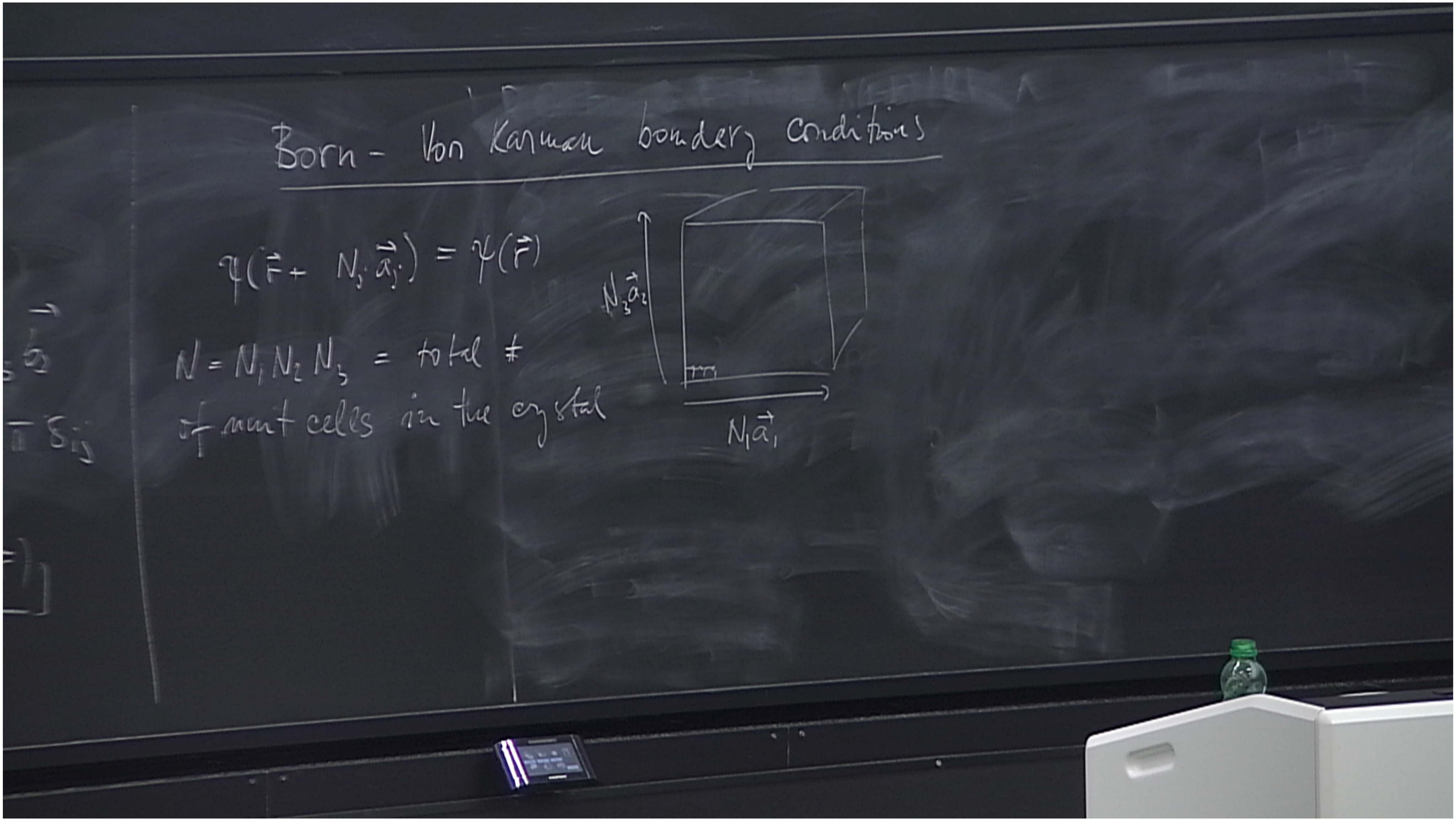
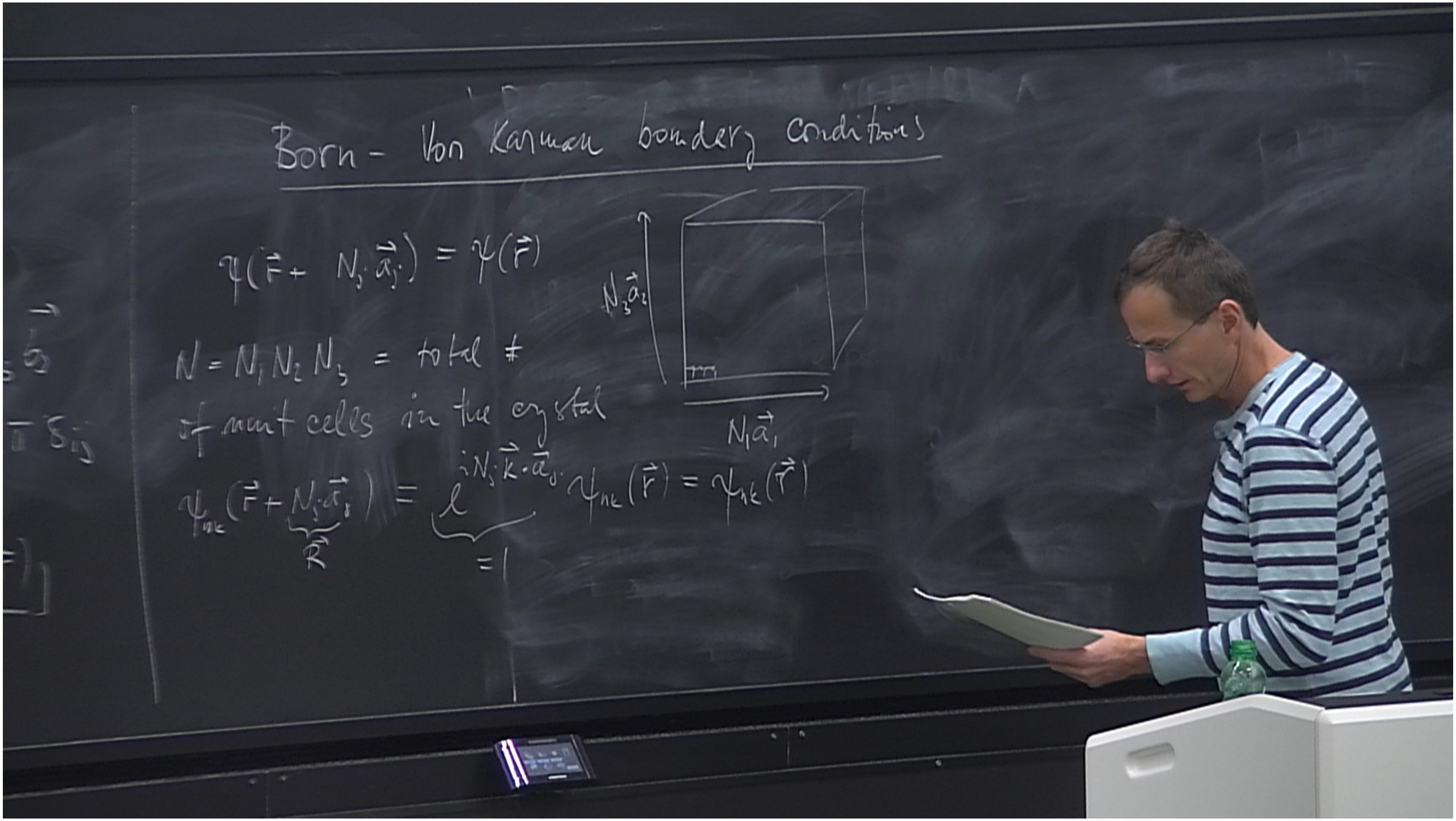
$$T_R\,\psi(\vec{r}) = \underline{\psi(\vec{r}+\vec{R})} = c(\vec{R})\,\psi(\vec{r}) = \underline{e^{i\vec{k}\cdot\vec{R}}\,\psi(\vec{r})},$$

Q.E.D.

Born - Von Karman boundary conditions

$$\psi(\vec{r} + N_j \vec{a}_j) = \psi(\vec{r})$$


Born - Von Karman bondery conditions
$\psi(\vec{r} + N_j \vec{a}_j) = \psi(\vec{r})$
$N = N_1 N_2 N_3$ = total # of unit cells in the crystal
$N_3 \vec{a}_2$
$N_1 \vec{a}_1$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$\psi_{nk}(\vec{r} + \underbrace{N_j \vec{a}_j}_{\vec{R}}) = \underbrace{e^{iN_j \vec{k}\cdot\vec{a}_j}}_{=1} \psi_{nk}(\vec{r}) = \psi_{nk}(\vec{r})$
$N_3 \vec{a}_2$
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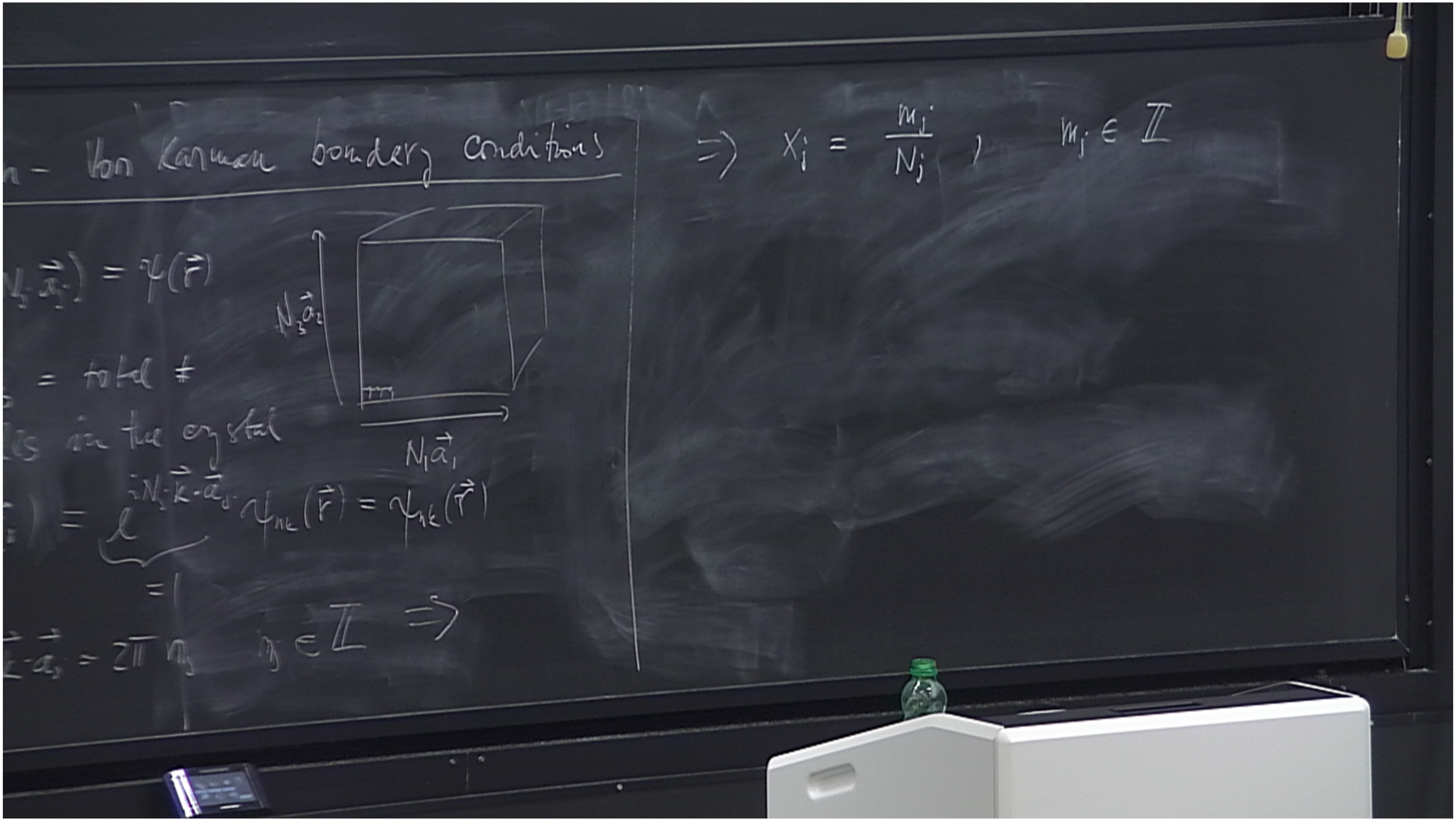
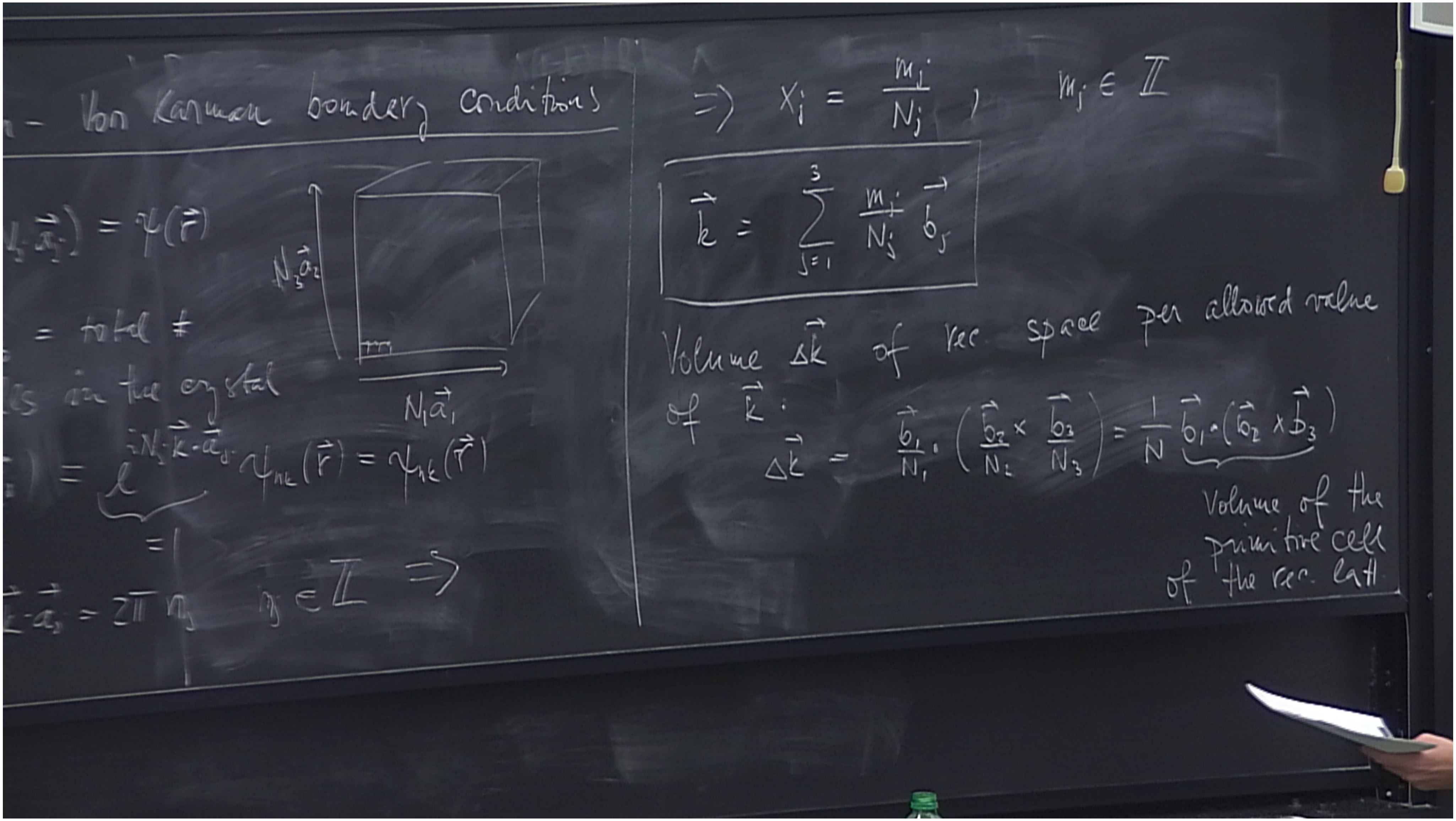
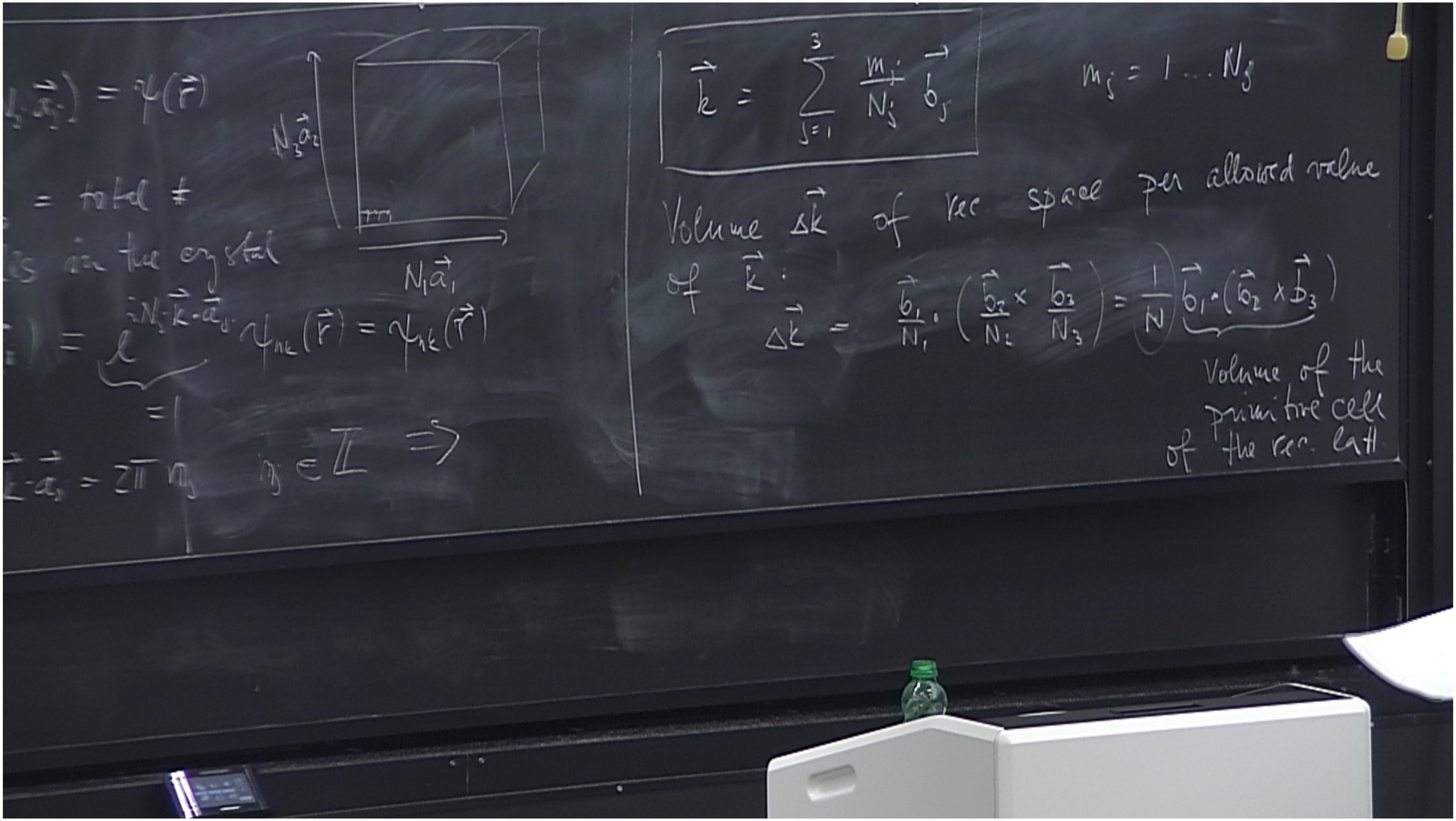

Von Karman bondery conditions
$\Rightarrow x_j = \frac{m_j}{N_j}$, $m_j \in \mathbb{Z}$
$= \psi(\vec{r})$
$N_2\vec{a}_2$
$N_1\vec{a}_1$
= total #
in the crystal
$= \underbrace{e^{iN_j \vec{k}\cdot\vec{a}_j}}_{=1} \psi_{nk}(\vec{r}) = \psi_{nk}(\vec{r})$
$\vec{k}\cdot\vec{a}_j = 2\pi m_j$ $m_j \in \mathbb{Z} \Rightarrow$


– Von Karman bondery conditions
$\Rightarrow x_j = \frac{m_j}{N_j}, \quad m_j \in \mathbb{Z}$
$\boxed{\vec{k} = \sum_{j=1}^{3} \frac{m_j}{N_j} \vec{b}_j}$
$= \psi(\vec{r})$
$N_3\vec{a}_3$
= total #
in the crystal
$N_1\vec{a}_1$
$= \underbrace{e^{iN_j \vec{k}\cdot\vec{a}_j}}_{=1} \psi_{nk}(\vec{r}) = \psi_{nk}(\vec{r})$
$\vec{k}\cdot\vec{a}_j = 2\pi n_j \quad n_j \in \mathbb{Z} \Rightarrow$
Volume $\Delta\vec{k}$ of rec. space per allowed value of $\vec{k}$:
$\Delta\vec{k} = \frac{\vec{b}_1}{N_1}\cdot\left(\frac{\vec{b}_2}{N_2}\times\frac{\vec{b}_3}{N_3}\right) = \frac{1}{N}\underbrace{\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)}$
Volume of the primitive cell of the rec. latt

with $u_{nk}(\vec{r}+\vec{R}) = u_{nk}(\vec{r})$.

- The # of allowed wave vectors $\vec{k}$ in a primitive cell of the rec. lattice is equal to the # of the unit cells of the crystal


$\vec{k} = \sum_{j=1}^{3} \frac{m_j}{N_j} \vec{b}_j$
$m_j = 1 \dots N_j$
Volume $\Delta\vec{k}$ of rec. space per allowed value of $\vec{k}$:
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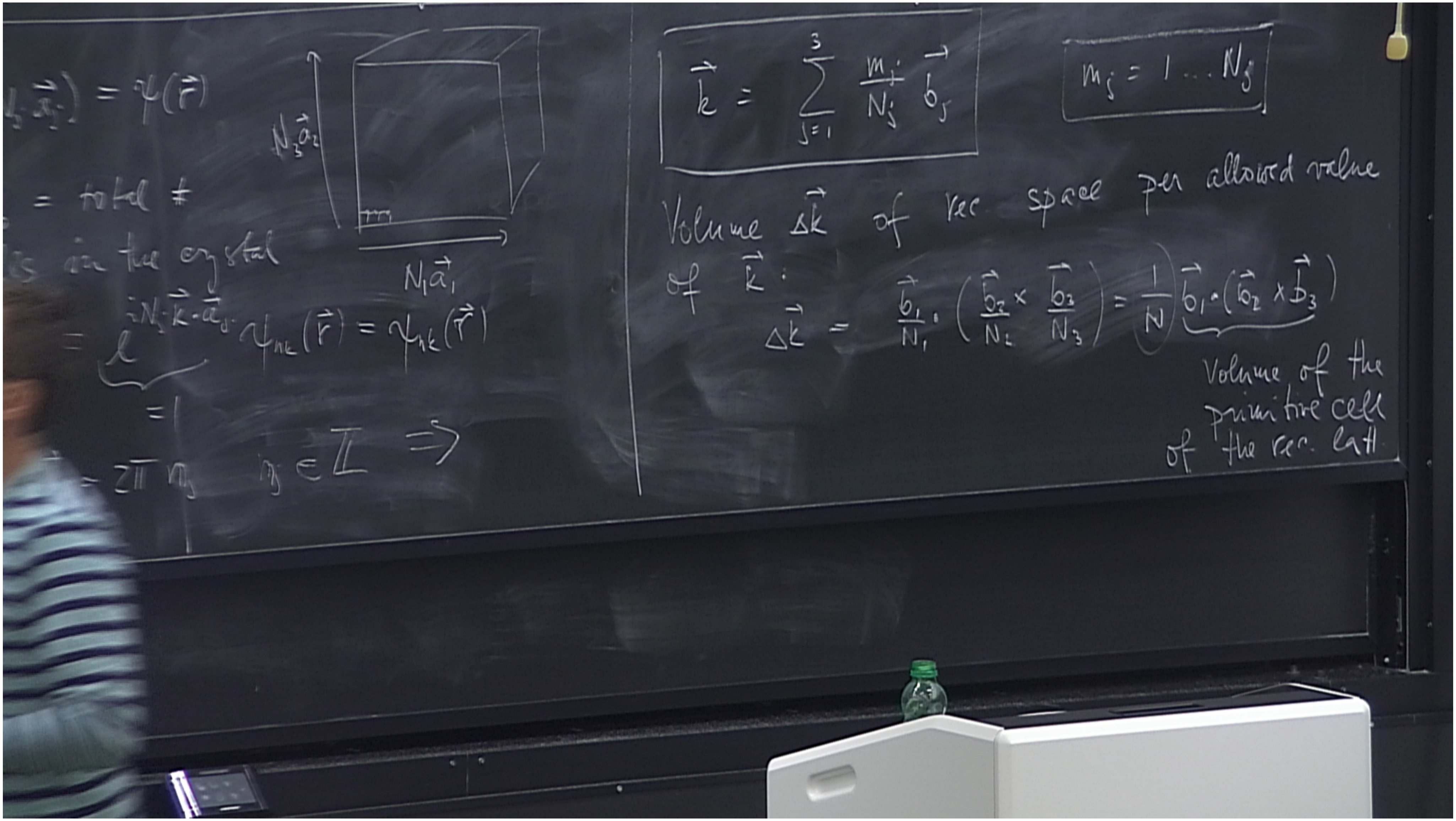
Volume of the primitive cell of the rec. latt.
$= \psi(\vec{r})$
= total #
in the crystal
$N_3\vec{a}_3$
$N_1\vec{a}_1$
$e^{iN_j \vec{k}\cdot\vec{a}_j}$
$\psi_{nk}(\vec{r}) = \psi_{nk}(\vec{r})$
$= 1$
$\vec{k}\cdot\vec{a}_j = 2\pi n_j$
$n_j \in \mathbb{Z} \Rightarrow$



= ψ(r)
= total #
in the crystal
N2 a2
N1 a1
ψnk(r) = ψnk(r)
= 1
= 2π nj
nj ∈ Z ⇒
k = Σ_{j=1}^{3} (mj / Nj) bj
mj = 1 ... Nj
Volume Δk of rec. space per allowed value
of k:
Δk = (b1 / N1) · ((b2 / N2) × (b3 / N3)) = (1 / N) b1 · (b2 × b3)
Volume of the
primitive cell
of the rec. latt.

General remarks

1. $\vec{k}$ is not a momentum,
it is a "crystal momentum"

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(1.) $\vec{k}$ is not a momentum,

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$$\hat{\vec{p}}\,\psi_{nk} = -i\hbar\vec{\nabla}\psi_{nk} = -i\hbar\vec{\nabla}\left(e^{i\vec{k}\cdot\vec{r}}u_{nk}(\vec{r})\right)$$

$$= \hbar\vec{k}\,\psi_{nk} + e^{i\vec{k}\vec{r}}\,\frac{\hbar}{i}\vec{\nabla}u_{nk}(\vec{r})$$

...momentum,

"...momentum"

$= -i\hbar \vec{\nabla}\left(e^{i\vec{k}\cdot\vec{r}} u_{nk}(\vec{r})\right)$

$e^{i\vec{k}\cdot\vec{r}} \frac{\hbar}{i} \vec{\nabla} u_{nk}(\vec{r})$

② The wavevector $\vec{k}$ can be always confined into the first Brillouin zone

...momentum,
"...momentum"

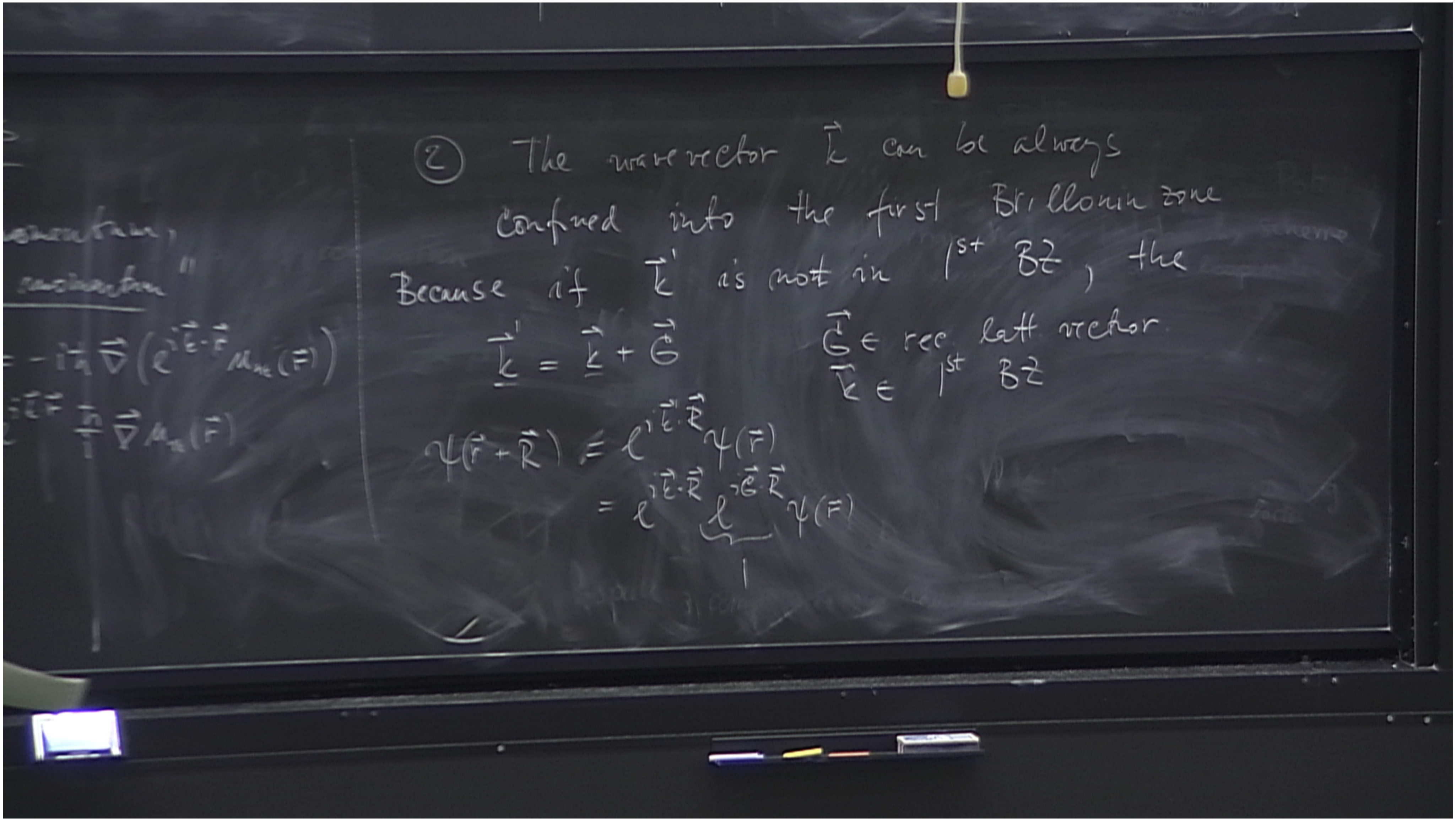
$= -i\hbar \vec{\nabla} \left(e^{i\vec{k}\cdot\vec{r}} u_{n\vec{k}}(\vec{r}) \right)$

$e^{i\vec{k}\cdot\vec{r}} \frac{\hbar}{i} \vec{\nabla} u_{n\vec{k}}(\vec{r})$

② The wavevector $\vec{k}$ can be always confined into the first Brillouin zone

Because if $\vec{k}'$ is not in 1^{st} BZ, then

$\vec{k}' = \vec{k} + \vec{G}$ $\vec{G} \in$ rec. latt. vector, $\vec{k} \in 1^{st}$ BZ



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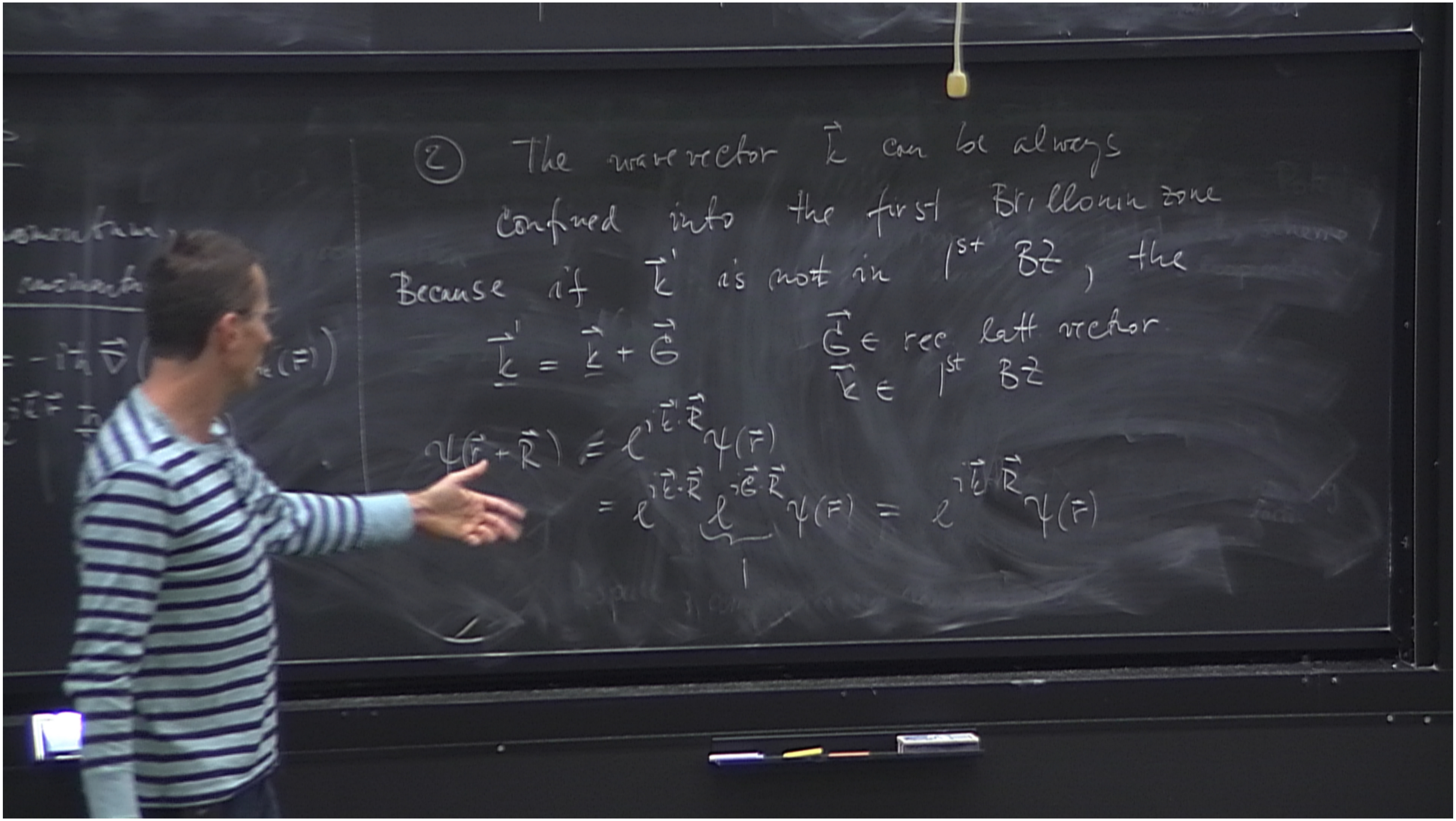
$\vec{G} \in$ rec. latt. vector
$\vec{k} \in 1^{st}$ BZ
$\psi(\vec{r}+\vec{R}) = e^{i\vec{k}'\cdot\vec{R}}\psi(\vec{r})$
$= e^{i\vec{k}\cdot\vec{R}} \underbrace{e^{i\vec{G}\cdot\vec{R}}}_{1} \psi(\vec{r})$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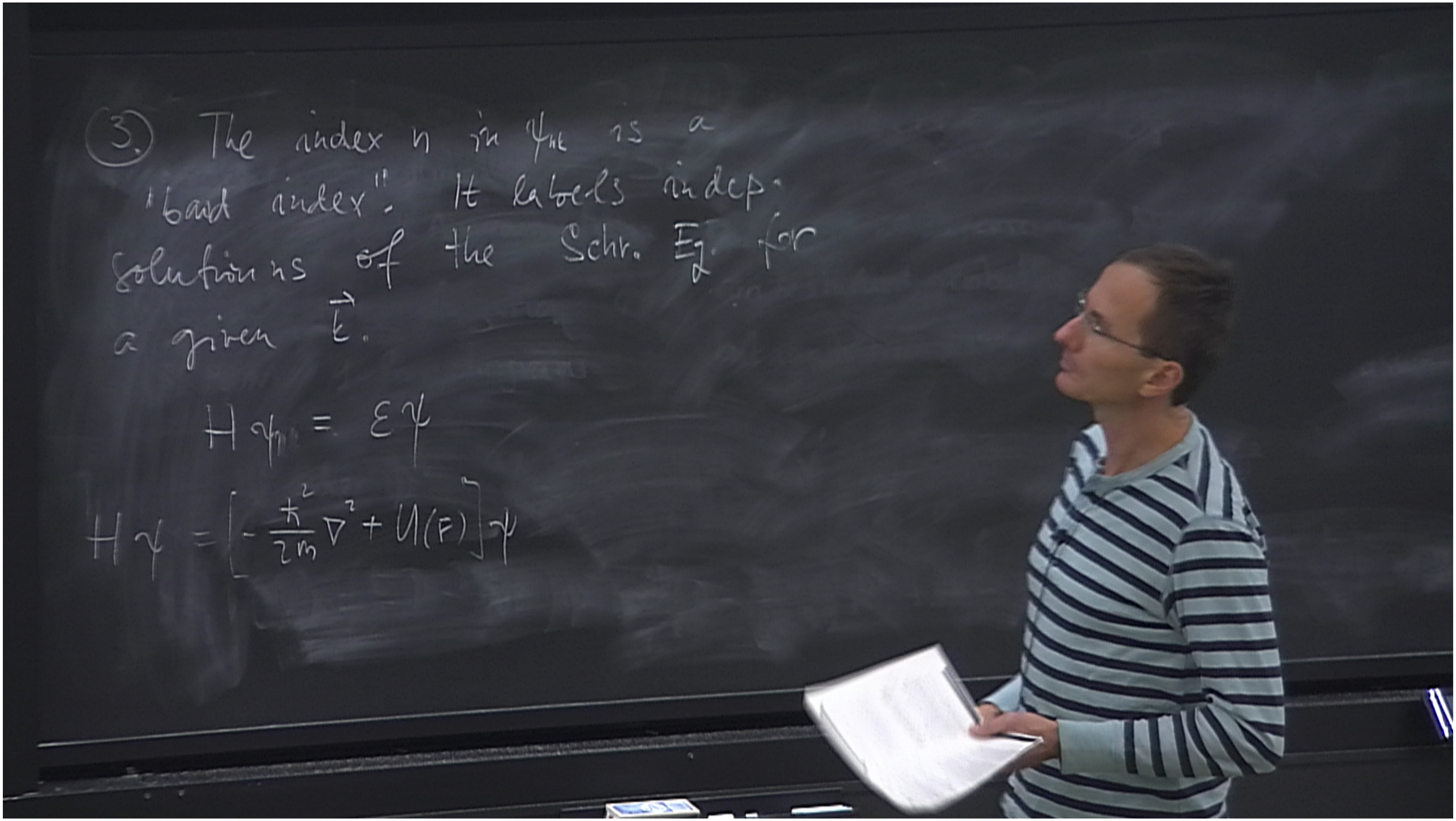
3. The index n in ψ_{nk} is a
"band index". It labels indep.
solutions of the Schr. Eq. for
a given $\vec{k}$.
$H\psi_{nk} = \varepsilon\psi$
$H\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right]\psi$

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$$H\psi_n = \varepsilon\psi$$

$$H\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right]\psi = \underbrace{e^{i\vec{k}\cdot\vec{r}}\left[\frac{\hbar^2}{2m}\left(-i\vec{\nabla}+\vec{k}\right)^2 + U(\vec{r})\right]u(\vec{r})}_{} = e^{i\vec{k}\cdot\vec{r}}\,\varepsilon\, u(\vec{r})$$

③ The index n in ψ_{nk} is a "band index". It labels indep. solutions of the Schr. Eq. for a given $\vec{k}$.

$$H\psi_{nk} = \varepsilon\psi$$

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(3.) The index n in ψ_{nk} is a "band index". It labels indep. solutions of the Schr. Eq. for a given $\vec{k}$.

$$H\psi_{nk} = \varepsilon\psi$$

$$H\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})\right]\psi = \underbrace{e^{i\vec{k}\cdot\vec{r}}\left[\frac{\hbar^2}{2m}\left(-i\vec{\nabla}+\vec{k}\right)^2 + U(\vec{r})\right]u(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\varepsilon\, u(\vec{r})}$$

– has infinitely many solutions for each $\vec{k}$, label by n.

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4. Electron in a Bloch state has non-vanishing average velocity

$$\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_k \varepsilon_n(\vec{k})$$

$$\left[(-i\vec{\nabla}+\vec{k})^2 + U(\vec{r})\right] u(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \varepsilon\, u(\vec{r})$$

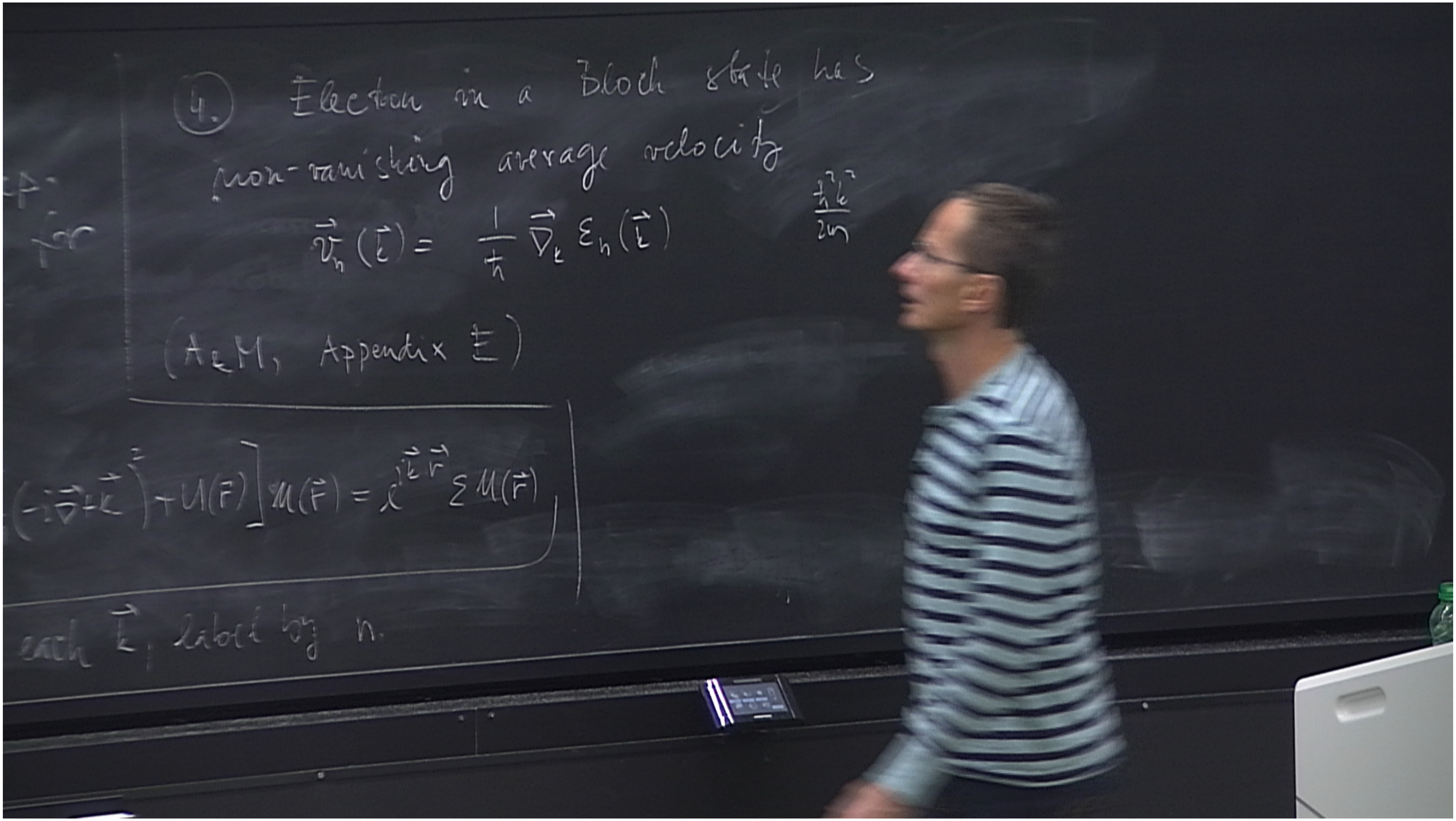
each $\vec{k}$, label by n.

④ Electron in a Bloch state has non-vanishing average velocity

$$\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_k \varepsilon_n(\vec{k}) \qquad \frac{\hbar^2 k^2}{2m}$$

$$\boxed{\left[\ldots(-i\vec{\nabla}+\vec{k})^2 + U(\vec{r})\right] u(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, \varepsilon\, u(\vec{r})}$$

each $\vec{k}$, label by n.


④ Electron in a Bloch state has
non-vanishing average velocity
$\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_k \varepsilon_n(\vec{k})$
$\frac{\hbar^2 k^2}{2m}$
(A&M, Appendix E)
$\left[\ldots(-i\vec{\nabla}+\vec{k})^2 + U(\vec{r})\right]u(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\,\varepsilon\, u(\vec{r})$
each $\vec{k}$, label by n.

…P:
for

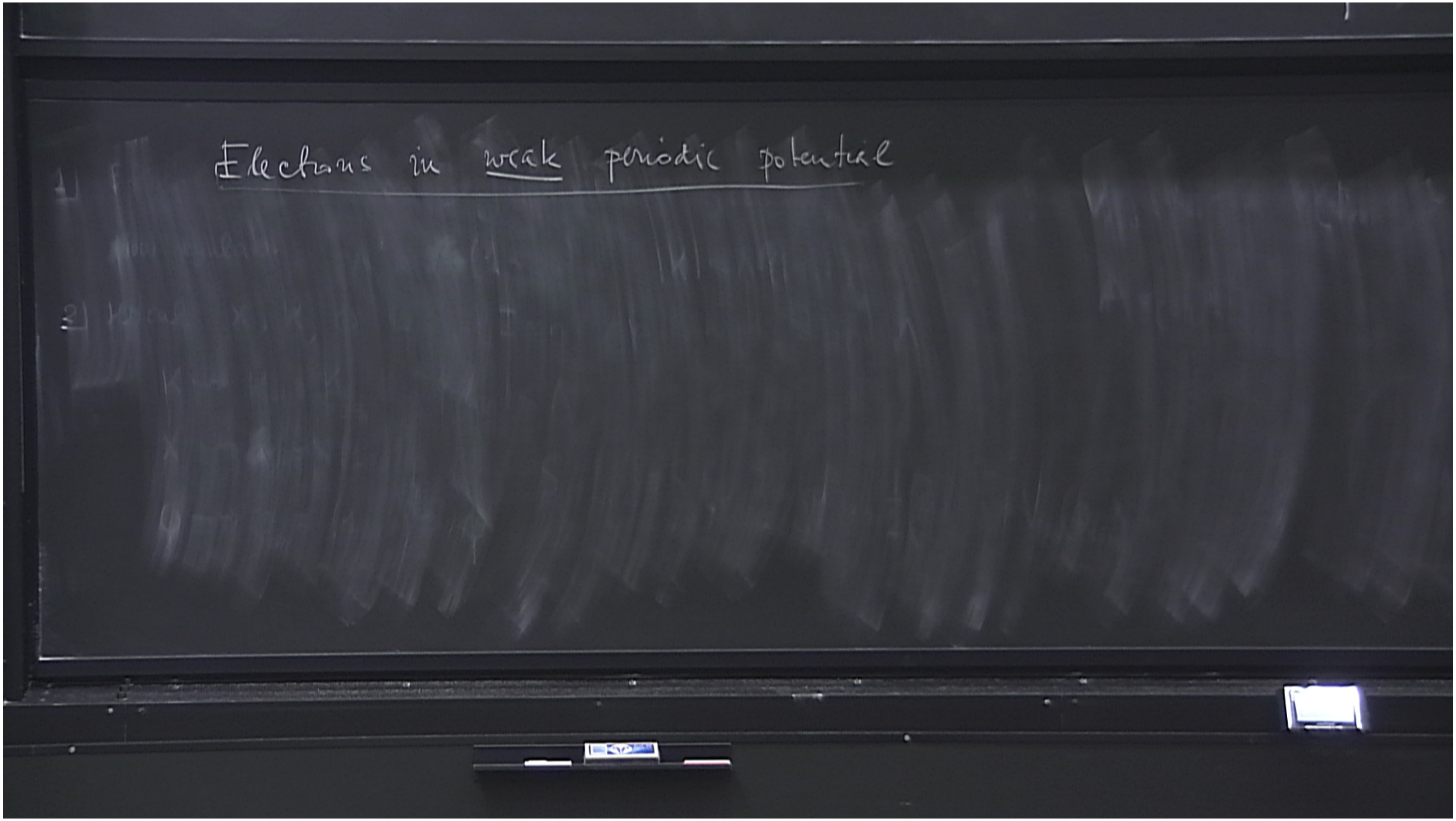
4. Electron in a Bloch state has non-vanishing average velocity

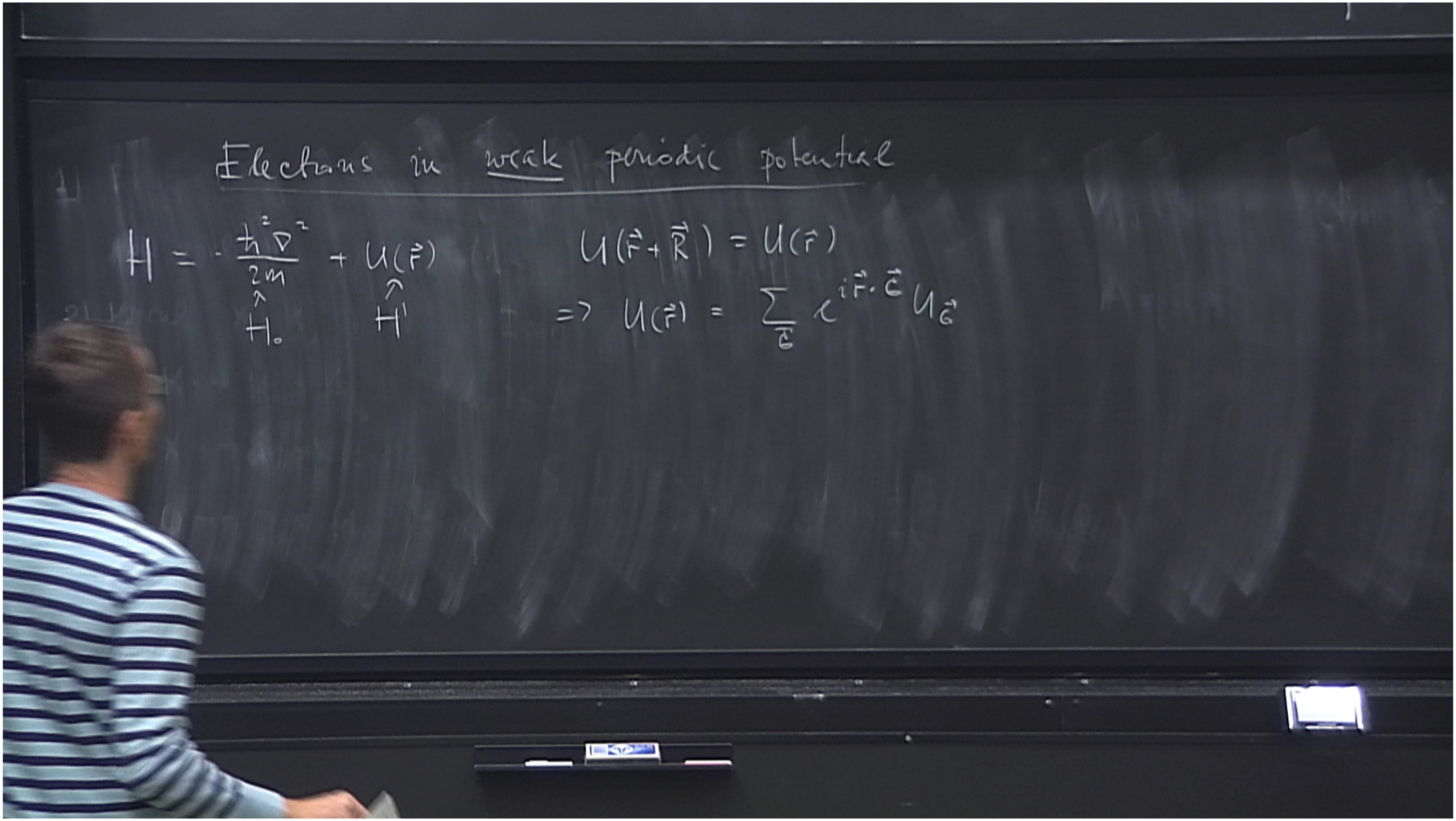
$$\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_k \varepsilon_n(\vec{k}) \qquad \frac{\hbar^2 k^2}{2m}$$

(A&M, Appendix E)

$$\left[(-i\vec{\nabla}+\vec{k})^2 + U(\vec{r})\right] u(\vec{r}) = e^{i\vec{k}\vec{r}}\, \varepsilon\, u(\vec{r})$$

each $\vec{k}$, label by n.


Electrons in weak periodic potential


Electrons in weak periodic potential
$H = -\frac{\hbar^2 \nabla^2}{2m} + U(\vec{r})$
$\hat{H}_0 \quad \hat{H}'$
$U(\vec{r} + \vec{R}) = U(\vec{r})$
$\Rightarrow U(\vec{r}) = \sum_{\vec{G}} e^{i\vec{r}\cdot\vec{G}} U_{\vec{G}}$

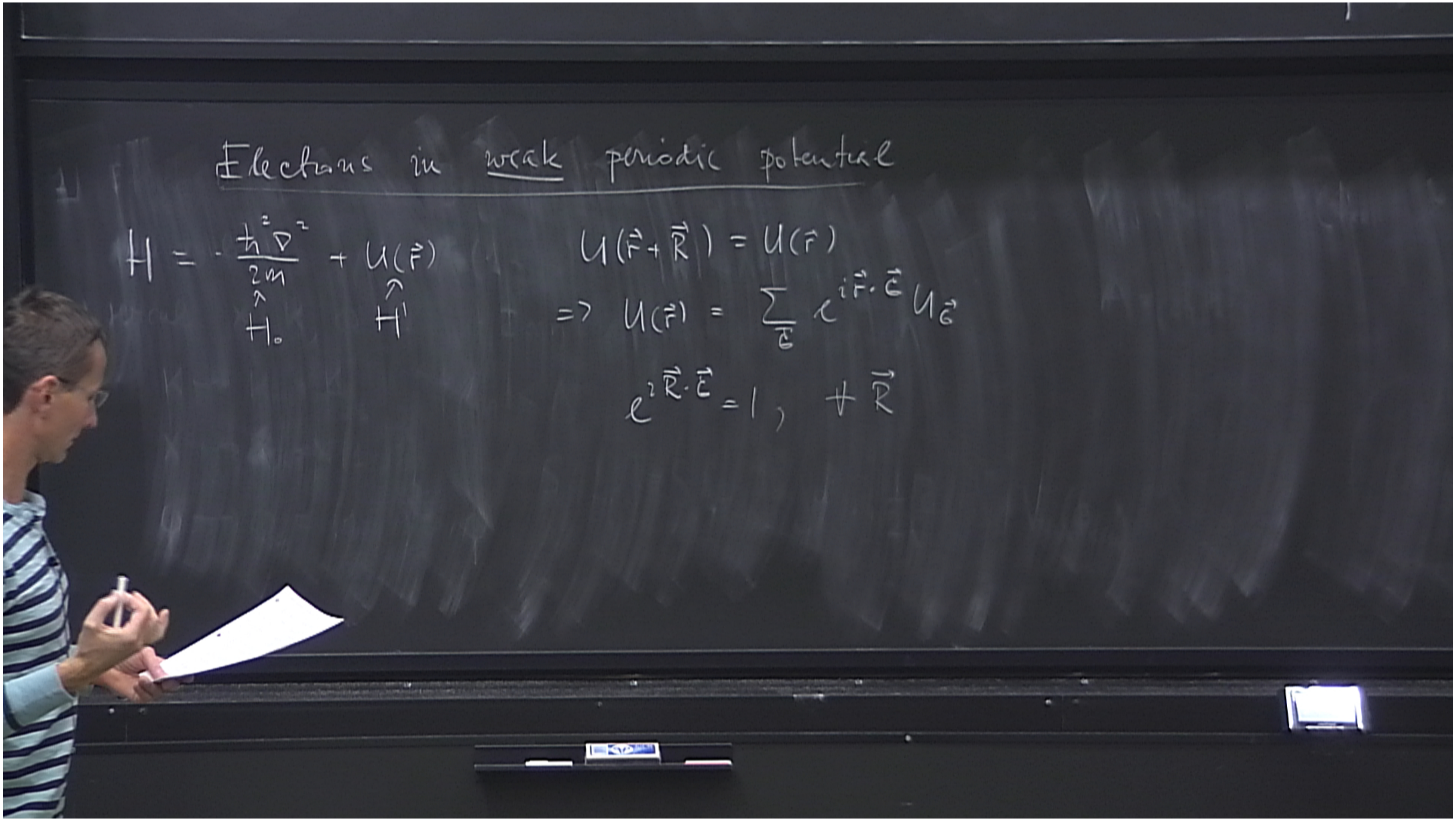
Electrons in weak periodic potential

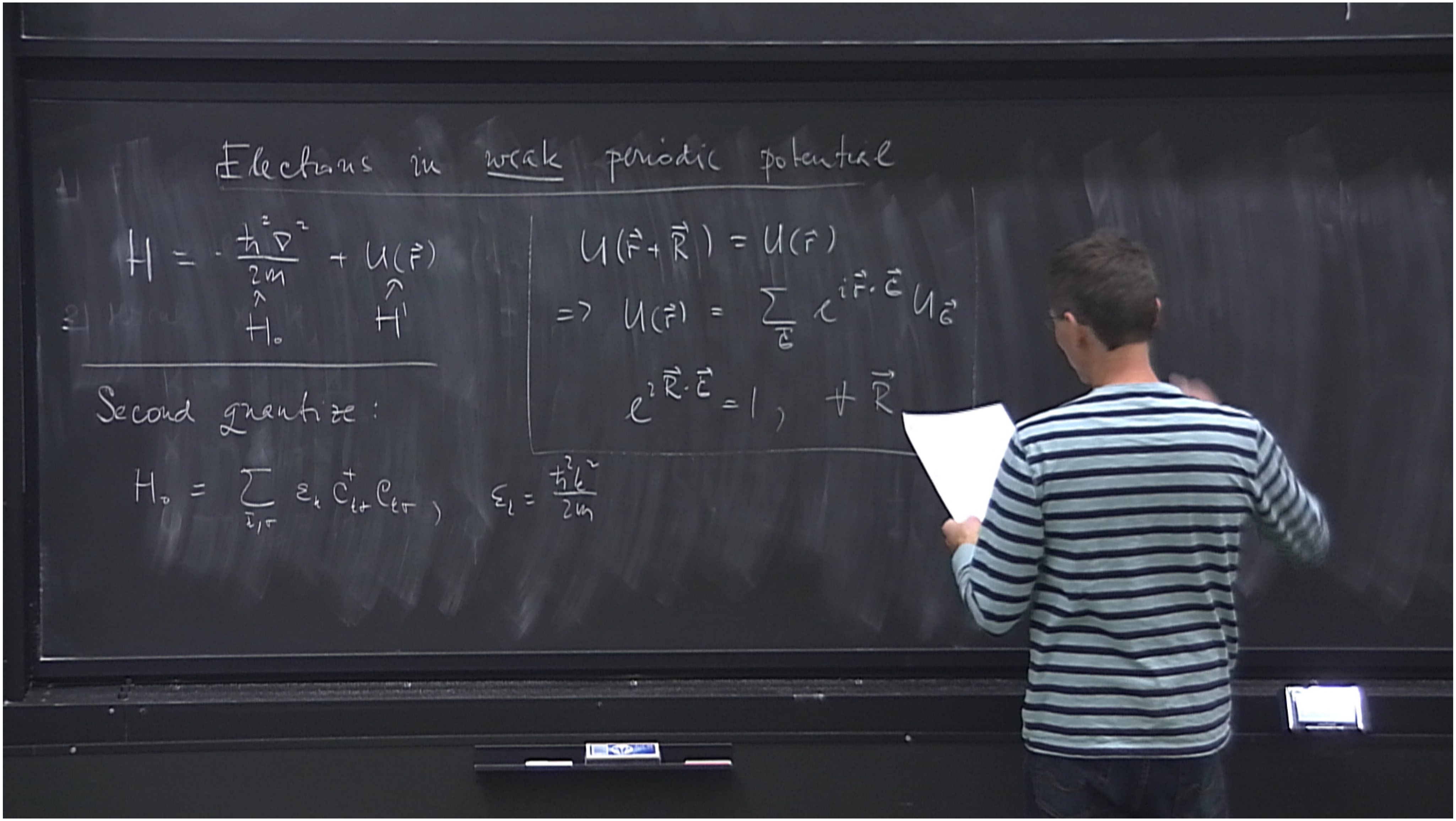
$$H = \underbrace{-\frac{\hbar^2\nabla^2}{2m}}_{H_0} + \underbrace{U(\vec r)}_{H'}$$

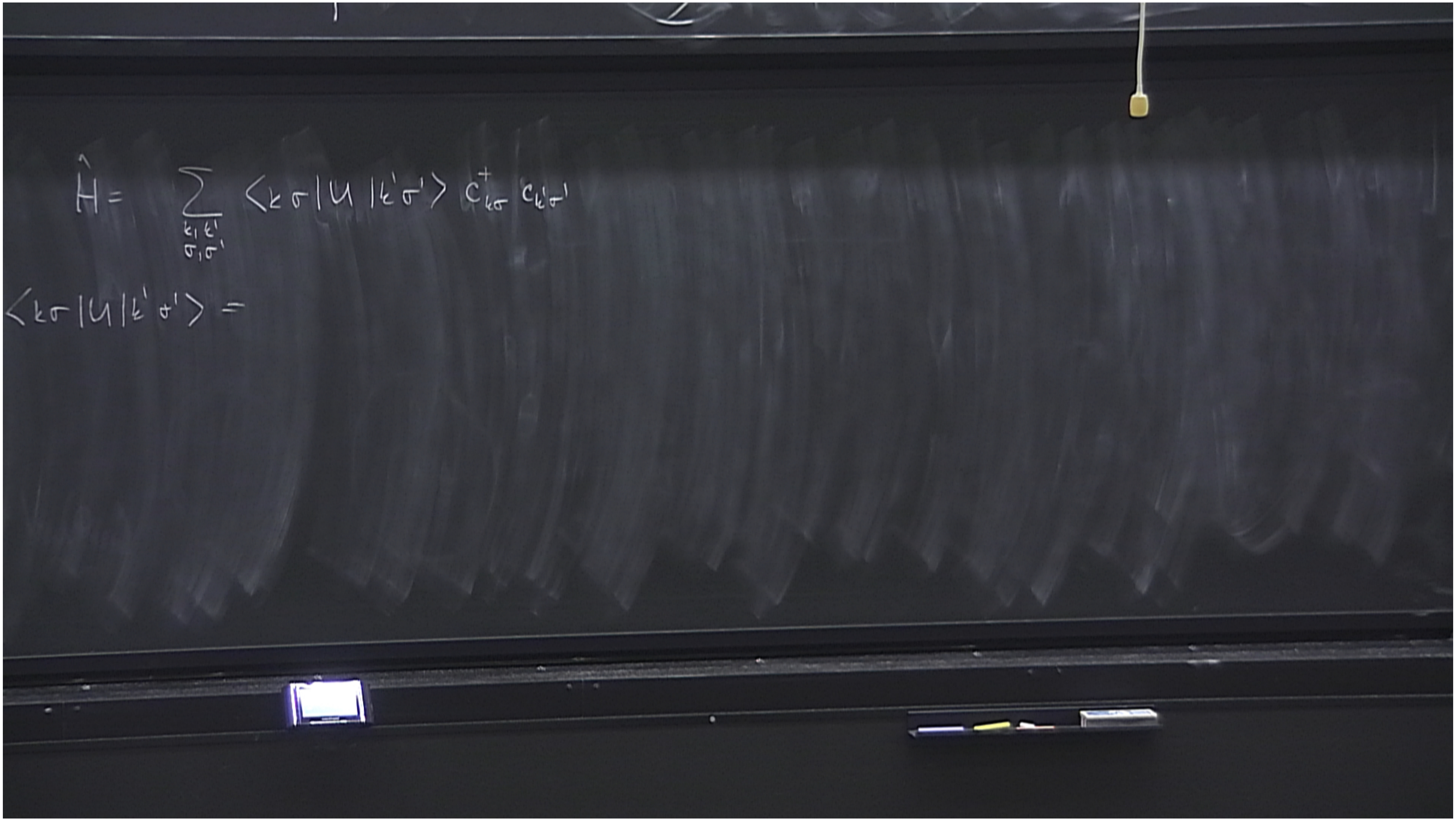
$$U(\vec r + \vec R) = U(\vec r)$$

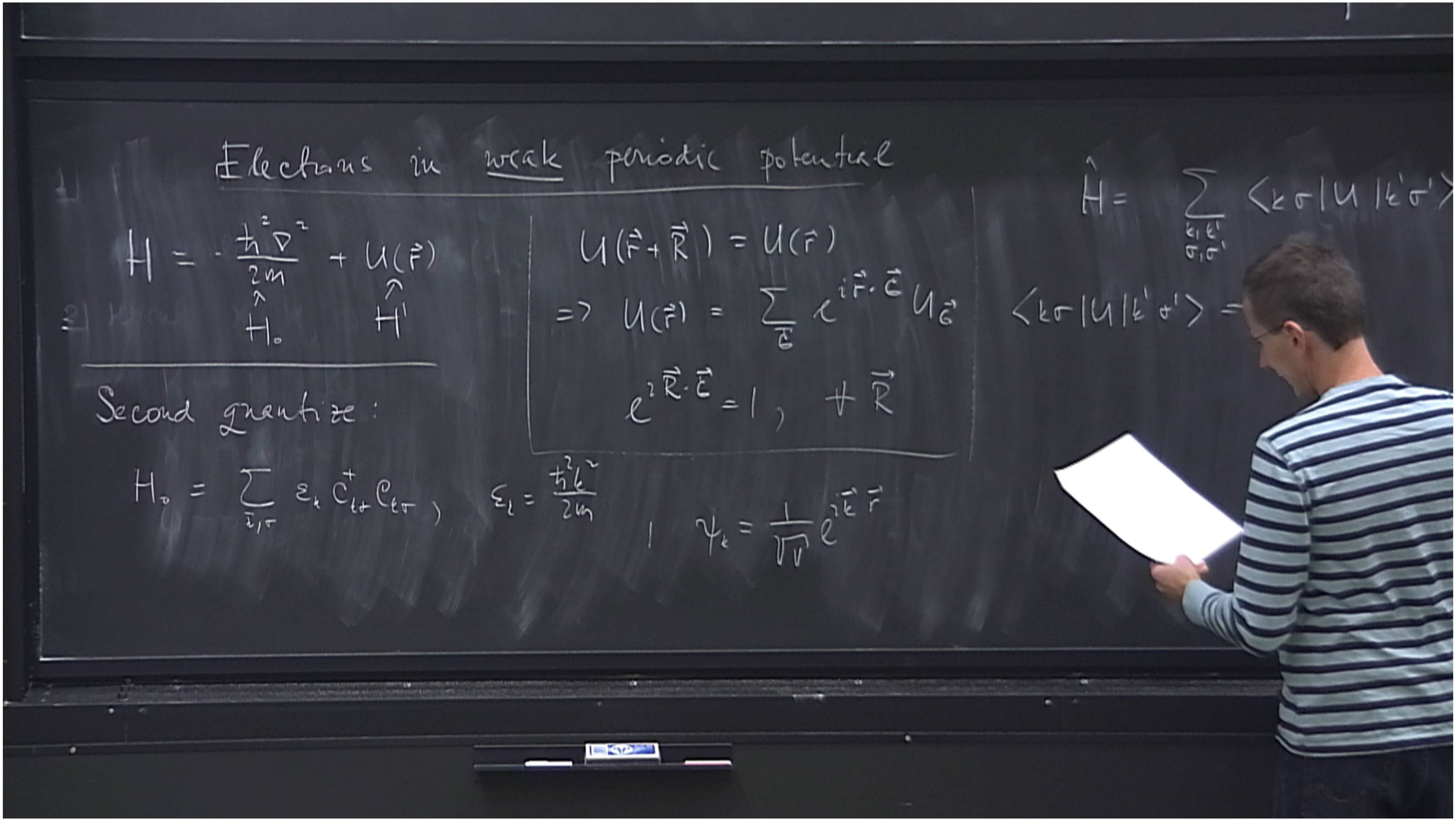
$$\Rightarrow U(\vec r) = \sum_{\vec G} e^{i\vec r\cdot\vec G}\, U_{\vec G}$$

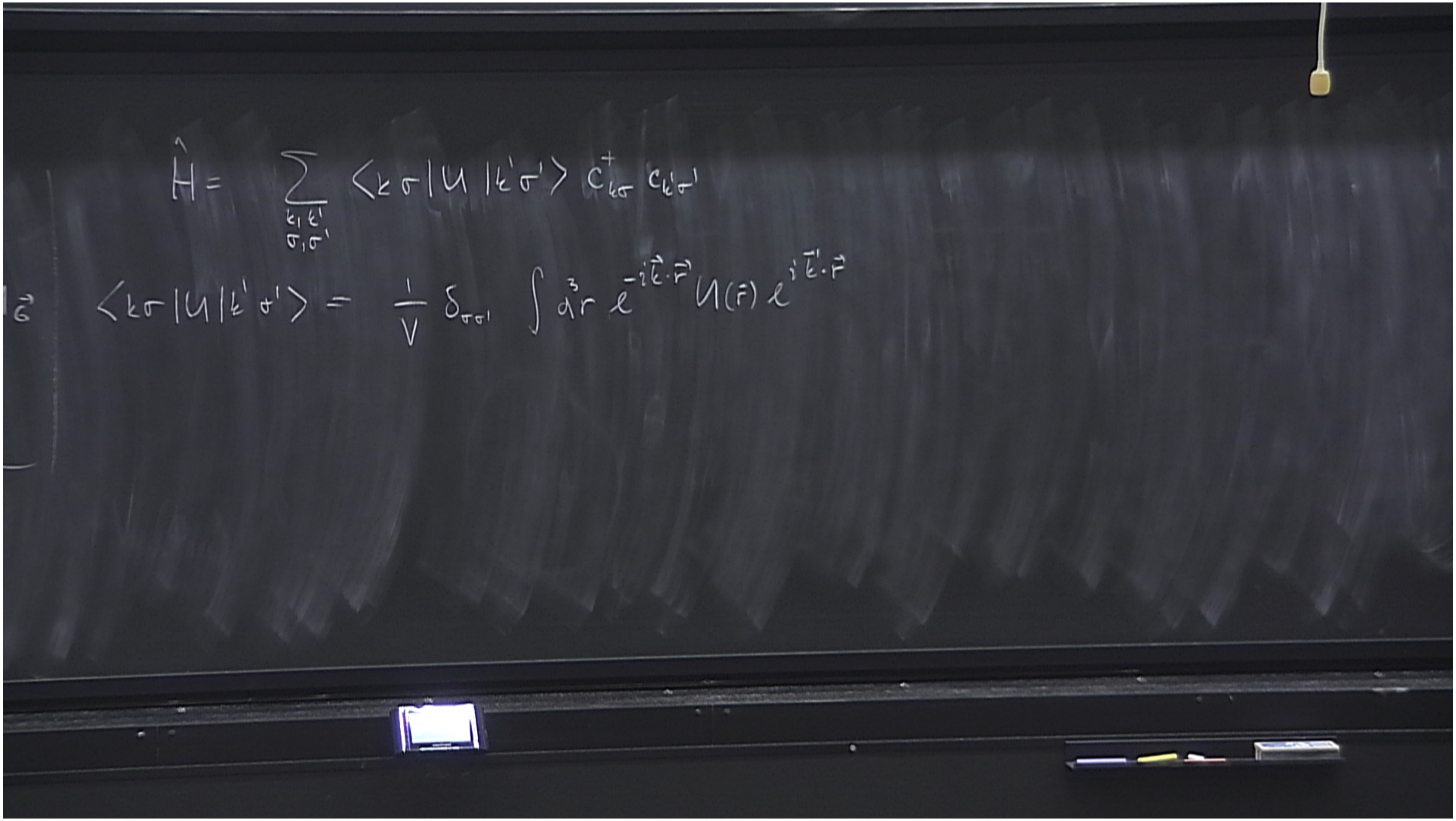
$$e^{i\vec R\cdot\vec G} = 1$$


Electrons in weak periodic potential
$H = -\frac{\hbar^2 \nabla^2}{2m} + U(\vec{r})$
$\hat{H}_0$ $\hat{H}'$
$U(\vec{r}+\vec{R}) = U(\vec{r})$
$\Rightarrow U(\vec{r}) = \sum_{\vec{G}} e^{i\vec{r}\cdot\vec{G}} U_{\vec{G}}$
$e^{i\vec{R}\cdot\vec{G}} = 1, \quad \forall \vec{R}$


Electrons in weak periodic potential
$H = -\frac{\hbar^2\nabla^2}{2m} + U(\vec{r})$
$\hat{H}_0 \quad \hat{H}'$
Second quantize:
$H_0 = \sum_{k,\sigma} \varepsilon_k c^{+}_{k\sigma} c_{k\sigma}, \quad \varepsilon_k = \frac{\hbar^2 k^2}{2m}$
$U(\vec{r}+\vec{R}) = U(\vec{r})$
$\Rightarrow U(\vec{r}) = \sum_{\vec{G}} e^{i\vec{r}\cdot\vec{G}} U_{\vec{G}}$
$e^{i\vec{R}\cdot\vec{G}} = 1, \quad \forall \vec{R}$


$\hat{H} = \sum_{\substack{k, k' \\ \sigma, \sigma'}} \langle k\sigma | U | k'\sigma' \rangle \, c^{+}_{k\sigma} c_{k'\sigma'}$
$\langle k\sigma | U | k'\sigma' \rangle =$


Electrons in weak periodic potential
H = -ħ²∇²/2m + U(r)
H₀ H'
Second quantize:
H₀ = Σ ε_k c⁺_kσ c_kσ , ε_k = ħ²k²/2m
U(r + R) = U(r)
=> U(r) = Σ_G e^{ir·G} U_G
e^{iR·G} = 1, ∀ R
ψ_k = 1/√V e^{ik·r}
Ĥ' = Σ ⟨kσ|U|k'σ'⟩
⟨kσ|U|k'σ'⟩ =



$\hat{H} = \sum_{k,k',\sigma,\sigma'} \langle k\sigma | U | k'\sigma'\rangle c^{+}_{k\sigma} c_{k'\sigma'}$
$\langle k\sigma | U | k'\sigma'\rangle = \frac{1}{V}\delta_{\sigma\sigma'} \int d^3r \, e^{-i\vec{k}\cdot\vec{r}} U(\vec{r}) e^{i\vec{k}'\cdot\vec{r}}$

$\vec{G}$

$$\hat{H} = \sum_{\substack{k,k' \\ \sigma,\sigma'}} \langle k\sigma|U|k'\sigma'\rangle \, c^{+}_{k\sigma} c_{k'\sigma'}$$

$$\langle k\sigma|U|k'\sigma'\rangle = \frac{1}{V}\delta_{\sigma\sigma'}\int d^3r \, e^{-i\vec{k}\cdot\vec{r}} U(\vec{r}) e^{i\vec{k}'\cdot\vec{r}}$$

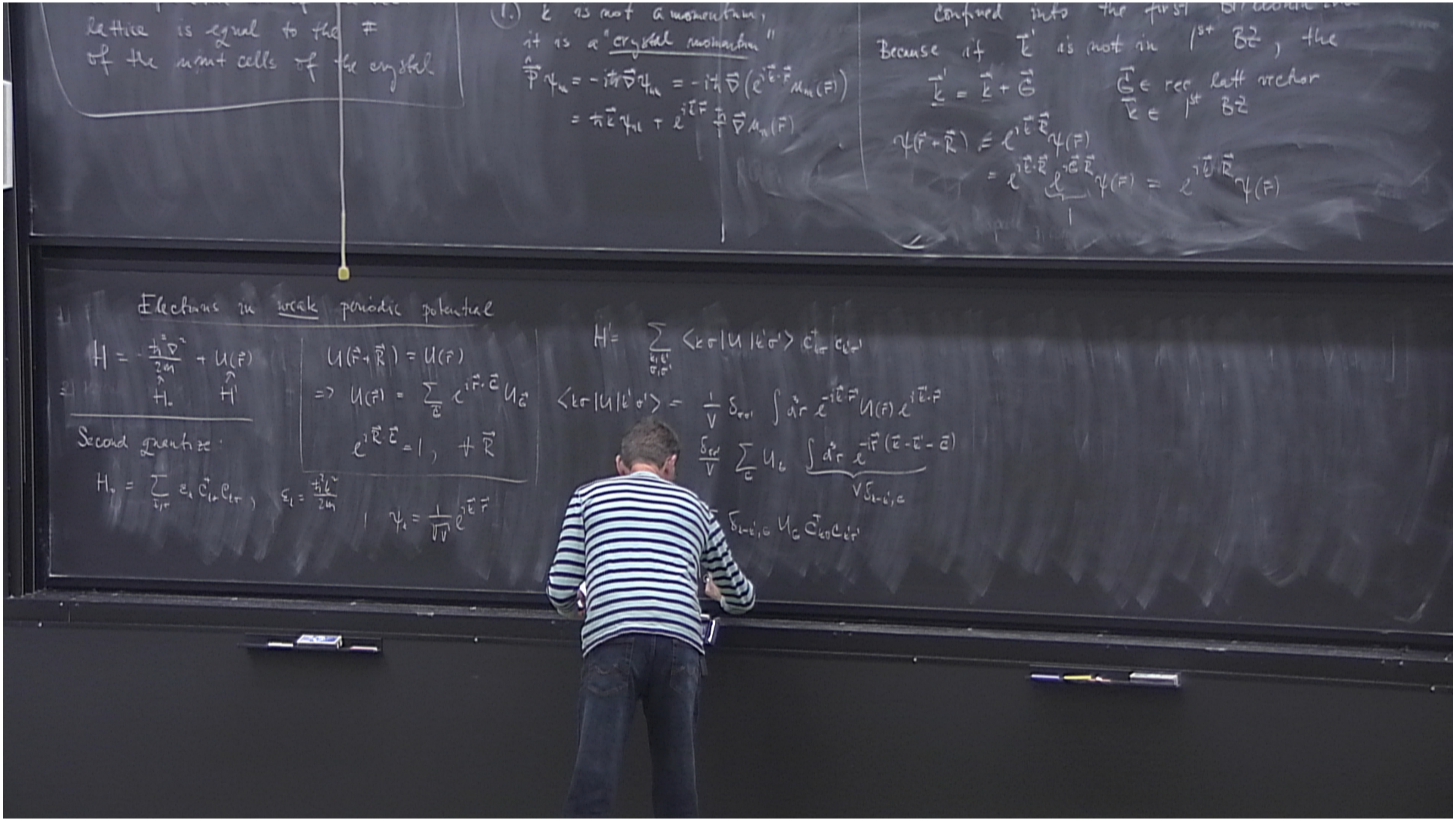
$$= \frac{\delta_{\sigma\sigma'}}{V}\sum_{G} U_G \int d^3r \, e^{-i\vec{r}(\vec{k}-\vec{k}'-\vec{G})}$$

$$H' = \sum_{\substack{k,k' \\ \sigma,\sigma'}} \langle k\sigma | U | k'\sigma' \rangle \, c^{\dagger}_{k\sigma} c_{k'\sigma'}$$

$$\langle k\sigma | U | k'\sigma' \rangle = \frac{1}{V} \delta_{\sigma\sigma'} \int d^3r \, e^{-i\vec{k}\cdot\vec{r}} \, U(\vec{r}) \, e^{i\vec{k}'\cdot\vec{r}}$$

$$= \frac{\delta_{\sigma\sigma'}}{V} \sum_{G} U_G \underbrace{\int d^3r \, e^{-i\vec{r}\cdot(\vec{k}-\vec{k}'-\vec{G})}}_{V\delta_{k-k',G}}$$

$$H' = \sum_{\substack{k k' \\ \sigma\sigma'}} \delta_{\sigma\sigma'} \sum_{G} \delta_{k-k',G} \, U_G \, c^{\dagger}_{k\sigma} c_{k'\sigma'}$$


lattice is equal to the #
of the unit cells of the crystal
1.) k is not a momentum,
it is a "crystal momentum"
confined into the first Brillouin zone
Because if k' is not in 1st BZ, the
G ∈ rec latt vector
k ∈ 1st BZ
Electrons in weak periodic potential
Second quantize:

$$H' = \sum_{\substack{k,k' \\ \sigma,\sigma'}} \langle k\sigma | U | k'\sigma' \rangle \, c^{\dagger}_{k\sigma} c_{k'\sigma'}$$

$$\langle k\sigma | U | k'\sigma' \rangle = \frac{1}{V} \delta_{\sigma\sigma'} \int d^3r \, e^{-i\vec{k}\cdot\vec{r}} U(\vec{r}) \, e^{i\vec{k}'\cdot\vec{r}}$$

$$= \frac{\delta_{\sigma\sigma'}}{V} \sum_{G} U_G \underbrace{\int d^3r \, e^{-i\vec{r}\cdot(\vec{k}-\vec{k}'-\vec{G})}}_{V\delta_{k-k',G}}$$

$$H' = \sum_{\substack{k\,k' \\ \sigma\sigma'}} \delta_{\sigma\sigma'} \sum_{G} \delta_{k-k',G} \, U_G \, c^{\dagger}_{k\sigma} c_{k'\sigma'}$$

$$\boxed{= \sum_{k,G,\sigma} U_{\vec{G}} \, c^{\dagger}_{\vec{k}+\vec{G},\sigma} c_{\vec{k}\sigma}}$$

$\langle k\sigma | U | k'\sigma' \rangle \, c^\dagger_{k\sigma} c_{k'\sigma'}$

$\frac{1}{V} \delta_{\sigma\sigma'} \int d^3r \, e^{-i\vec{k}\cdot\vec{r}} U(\vec{r}) \, e^{i\vec{k}'\cdot\vec{r}}$

$\frac{\delta_{\sigma\sigma'}}{V} \sum_G U_G \underbrace{\int d^3r \, e^{-i\vec{r}\,(\vec{k}-\vec{k}'-\vec{G})}}_{V\delta_{k-k',G}}$

$\sum_G \delta_{k-k',G} \, U_G \, c^\dagger_{k\sigma} c_{k'\sigma'}$

$U_{\vec{G}} \, c^\dagger_{\vec{k}+\vec{G},\sigma} c_{\vec{k}\sigma}$

1) Consider a 1D system

2) Supress the spin index

$\langle k\sigma | U | k'\sigma' \rangle \, c^{\dagger}_{k\sigma} c_{k'\sigma'}$

$\frac{1}{V} \delta_{\sigma\sigma'} \int d^3r \, e^{-i\vec{k}\cdot\vec{r}} U(\vec{r}) \, e^{i\vec{k}'\cdot\vec{r}}$

$\frac{\delta_{\sigma\sigma'}}{V} \sum_{G} U_G \underbrace{\int d^3r \, e^{-i\vec{r}(\vec{k}-\vec{k}'-\vec{G})}}_{V\delta_{k-k',G}}$

$\sum_{G} \delta_{k-k',G} U_G c^{\dagger}_{k\sigma} c_{k'\sigma'}$

$U_G \, c^{\dagger}_{\vec{k}+\vec{G},\sigma} c_{k\sigma}$

1) Consider a 1D system

2) Supress the spin index

3) Assume $U_{\vec{G}=0} = 0$

$k\sigma | U | k'\sigma' \rangle \, c^\dagger_{k\sigma} c_{k'\sigma'}$

$\frac{1}{V} \delta_{\sigma\sigma'} \int d^3r \, e^{-i\vec{k}\cdot\vec{r}} U(\vec{r}) \, e^{i\vec{k}'\cdot\vec{r}}$

$\frac{\delta_{\sigma\sigma'}}{V} \sum_G U_G \underbrace{\int d^3r \, e^{-i\vec{r}(\vec{k}-\vec{k}'-\vec{G})}}_{V\delta_{k-k',G}}$

$\sum_G \delta_{k-k',G} U_G \, c^\dagger_{k\sigma} c_{k'\sigma'}$

$U_{\vec{G}} \, c^\dagger_{\vec{k}+\vec{G},\sigma} c_{\vec{k}\sigma}$

1) Consider a 1D system

2) Supress the spin index

3) Assume $U_{\vec{G}=0} = 0$

Do perturbation theory in U

$|k\rangle = c^\dagger_k |0\rangle$

$$\langle k\sigma|U|k'\sigma'\rangle\, c^\dagger_{k\sigma} c_{k'\sigma'}$$

$$\frac{1}{V}\delta_{\sigma\sigma'}\int d^3r\, e^{-i\vec{k}\cdot\vec{r}}\, U(\vec{r})\, e^{i\vec{k}'\cdot\vec{r}}$$

$$\frac{\delta_{\sigma\sigma'}}{V}\sum_{G} U_G \underbrace{\int d^3r\, e^{-i\vec{r}\,(\vec{k}-\vec{k}'-\vec{G})}}_{V\delta_{k-k',G}}$$

$$\sum_{G}\delta_{k-k',G}\, U_G\, c^\dagger_{k\sigma} c_{k'\sigma'}$$

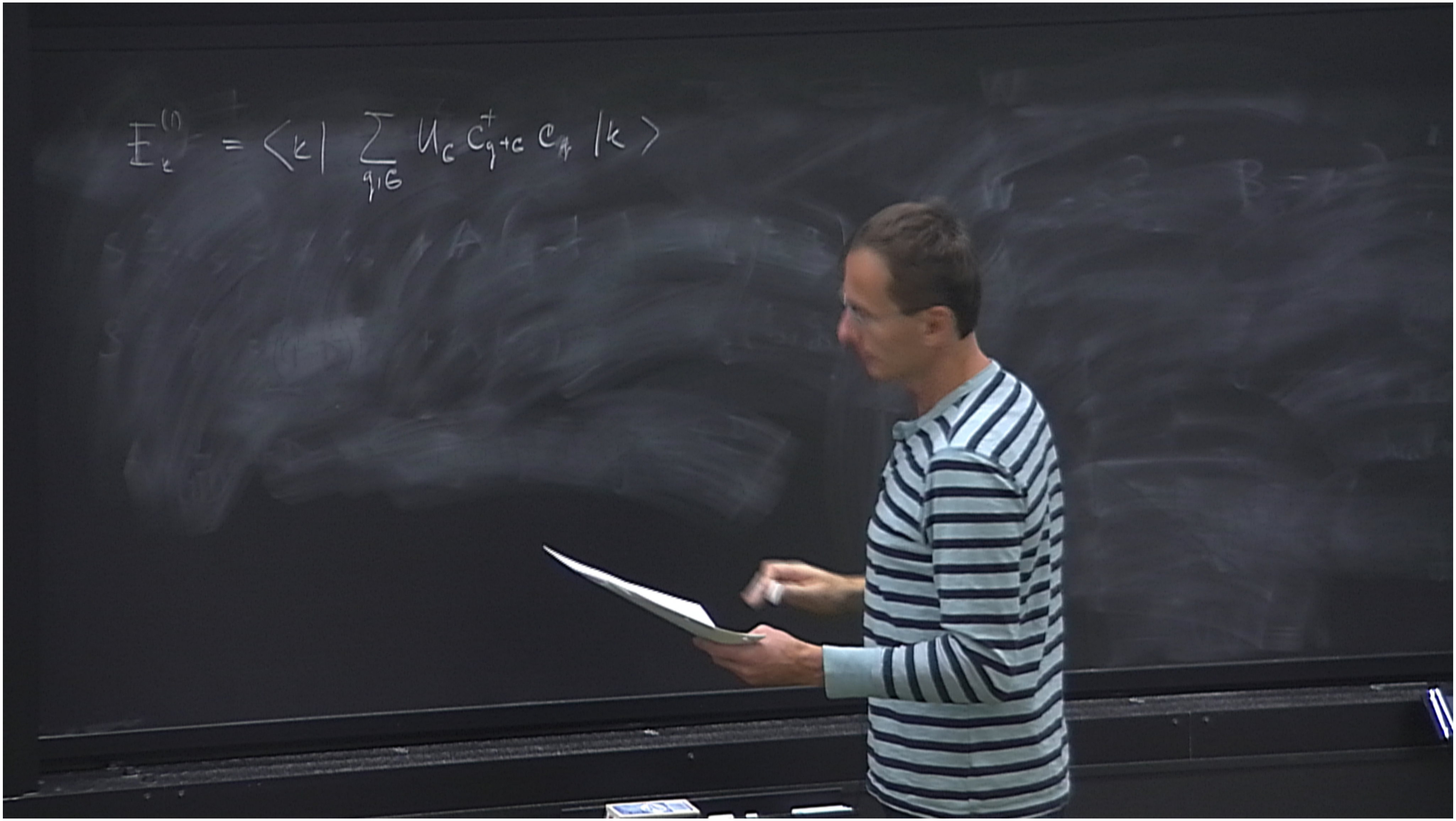
$$\boxed{U_{\vec{G}}\, c^\dagger_{\vec{k}+\vec{G},\sigma}\, c_{\vec{k}\sigma}}$$

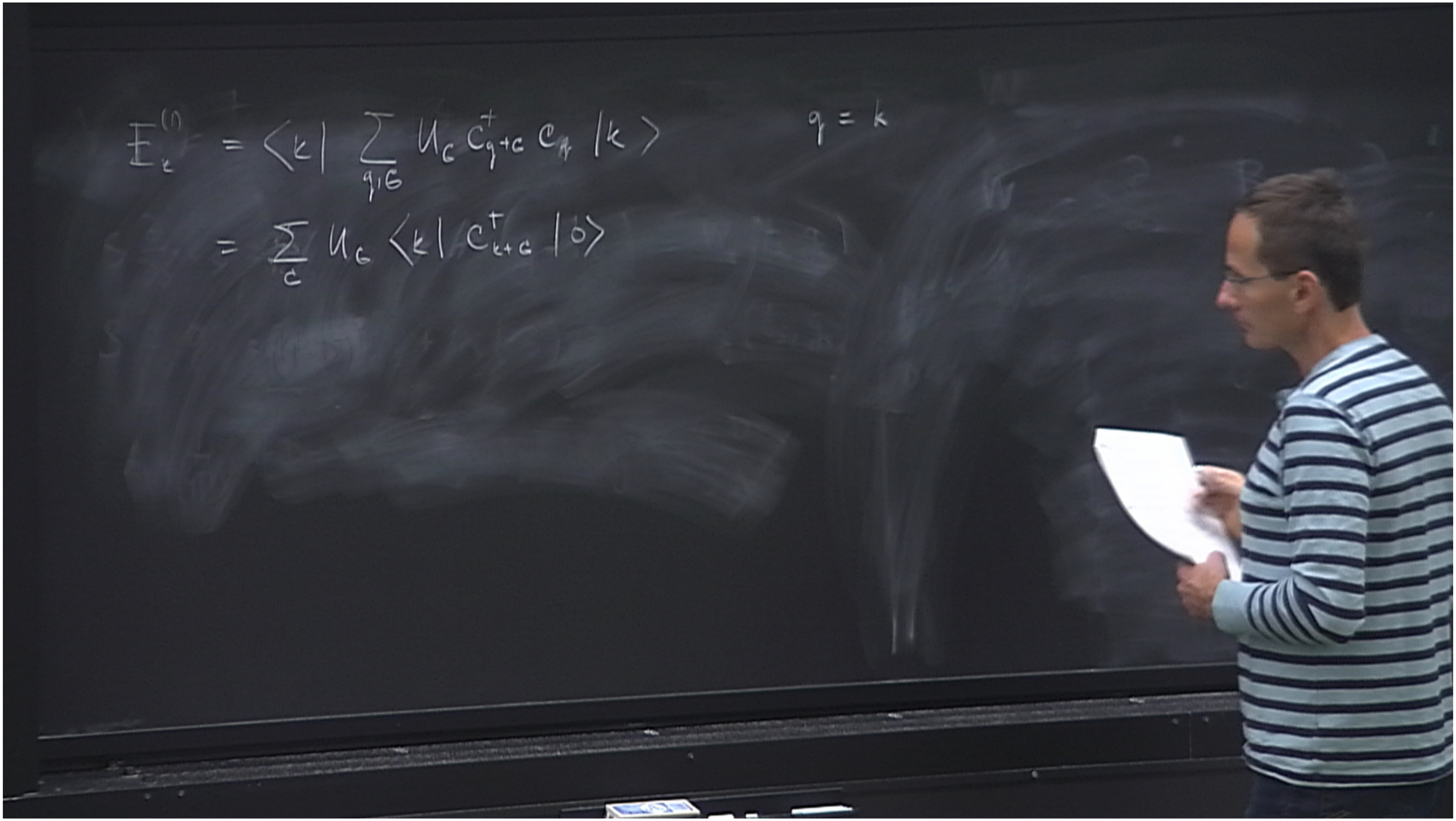
1) Consider a 1D system
2) Supress the spin index
3) Assume $U_{\vec{G}=0} = 0$

Do perturbation theory in H'

$$|k\rangle = c^\dagger_k|0\rangle$$

$$E^{(0)}_k = \varepsilon_k$$


$E_k^{(1)} = \langle k | \sum_{q,G} U_G c^\dagger_{q+G} c_q | k \rangle$


$E_k^{(1)} = \langle k | \sum_{q,G} U_G c^{\dagger}_{q+G} c_q | k \rangle$
$q = k$
$= \sum_G U_G \langle k | c^{\dagger}_{k+G} | 0 \rangle$

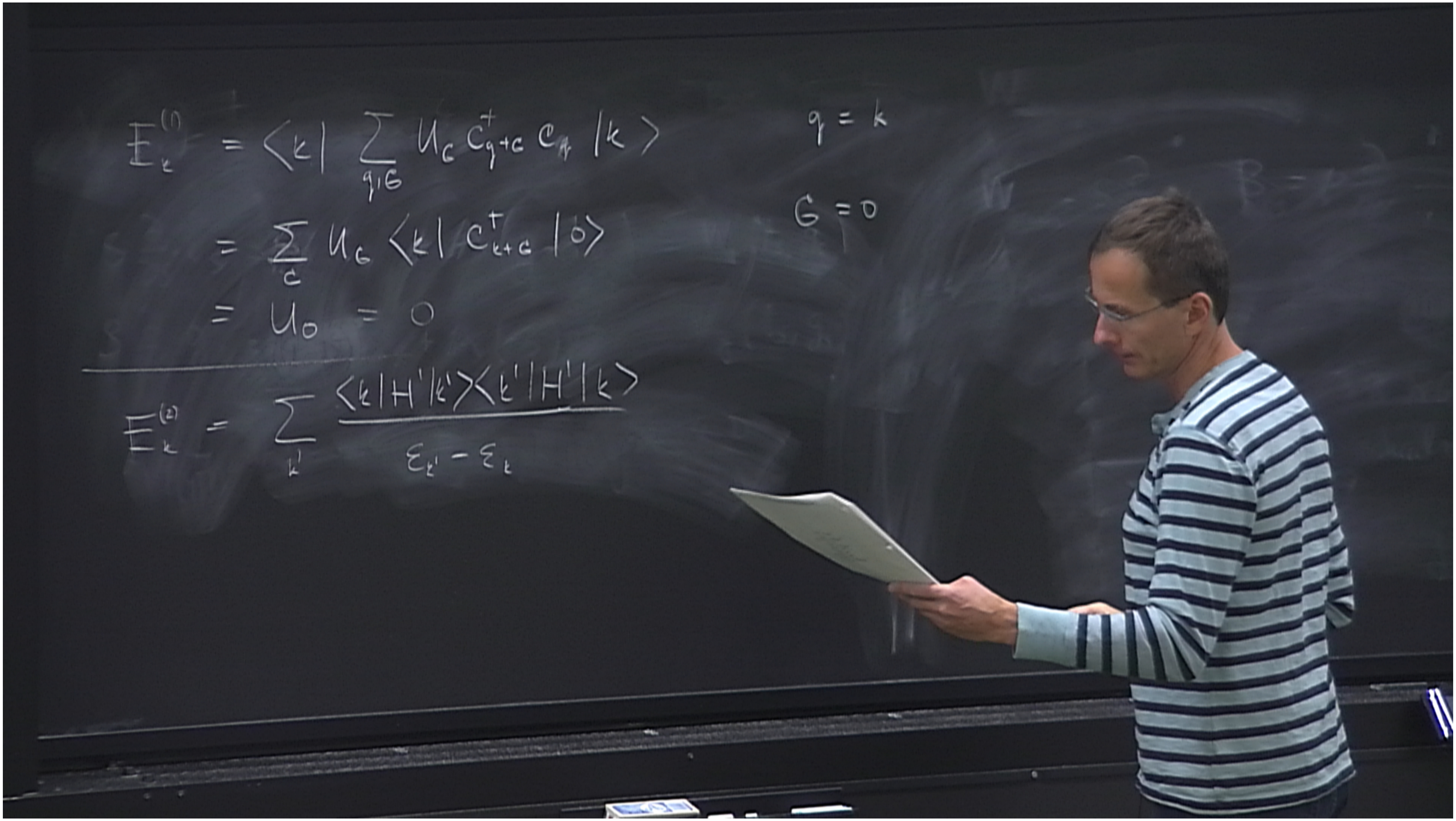
$$E_k^{(1)} = \langle k | \sum_{q,G} U_G \, c^\dagger_{q+G} \, c_q \, | k \rangle$$

$$= \sum_G U_G \, \langle k | \, c^\dagger_{k+G} \, | 0 \rangle$$

$$= U_0$$

$q = k$

$G = 0$


$E_k^{(1)} = \langle k | \sum_{q,G} U_G c^\dagger_{q+G} c_q | k \rangle$
$q = k$
$G = 0$
$= \sum_G U_G \langle k | c^\dagger_{k+G} | 0 \rangle$
$= U_0 = 0$
$E_k^{(2)} = \sum_{k'} \frac{\langle k | H' | k' \rangle \langle k' | H' | k \rangle}{\varepsilon_{k'} - \varepsilon_k}$

$$E_k^{(1)} = \langle k | \sum_{q,G} U_G\, c^\dagger_{q+G}\, c_q\, | k \rangle$$

$q = k$

$G = 0$

$$= \sum_G U_G \langle k | c^\dagger_{k+G} | 0 \rangle$$

$$= U_0 = 0$$

$$E_k^{(2)} = \sum_{k'} \frac{\langle k | H' | k' \rangle \langle k' | H' | k \rangle}{\varepsilon_{k'} - \varepsilon_k}$$

$$\langle k | H' | k' \rangle = \sum_G U_G\, \delta_{k, k'+G}$$

$$E_k^{(1)} = \langle k| \sum_{q,G} U_G\, c^\dagger_{q+G}\, c_q\, |k\rangle$$

$$= \sum_G U_G \langle k|\, c^\dagger_{k+G}\, |0\rangle$$

$$= U_0 = 0$$

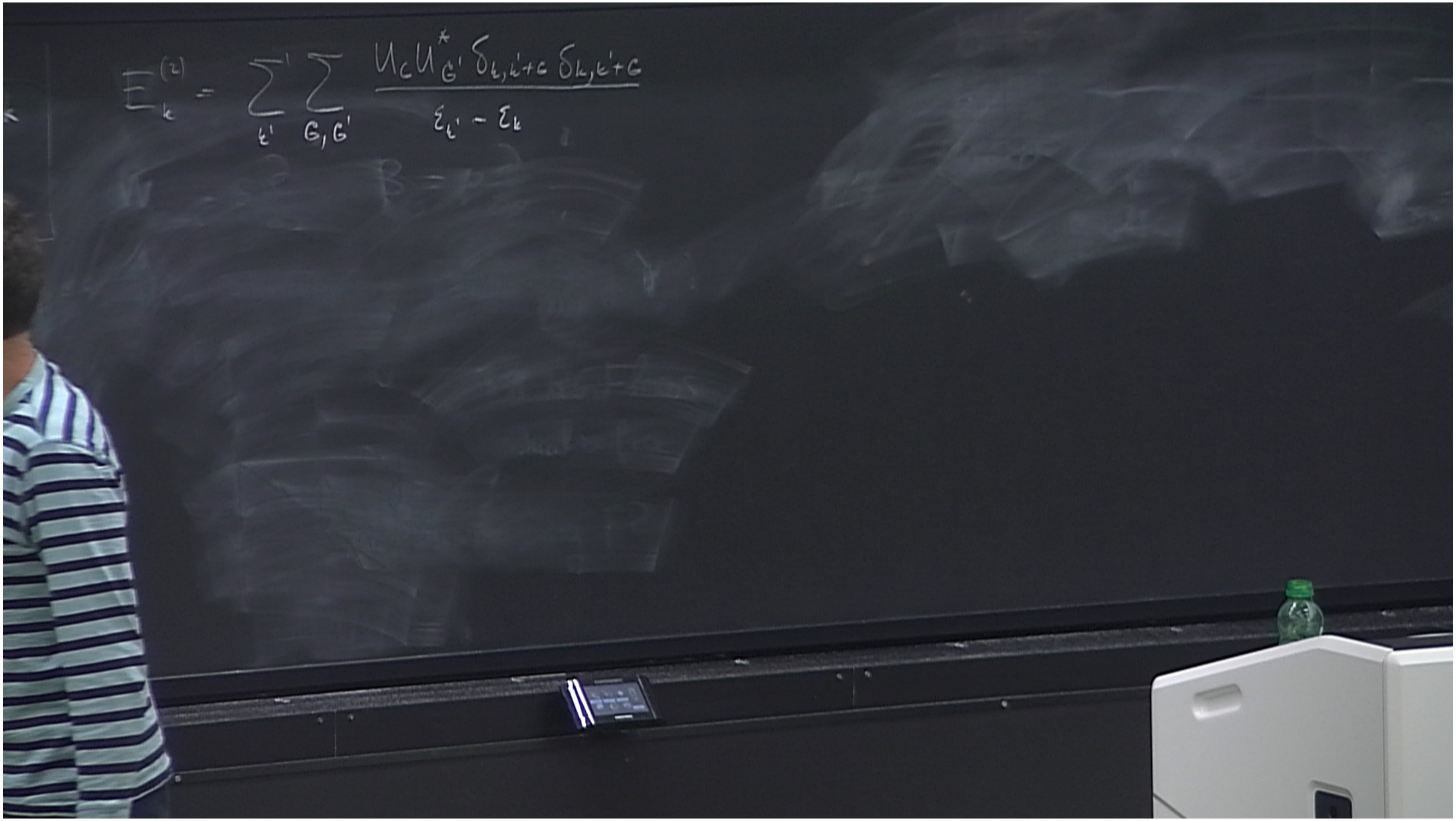
$q = k$

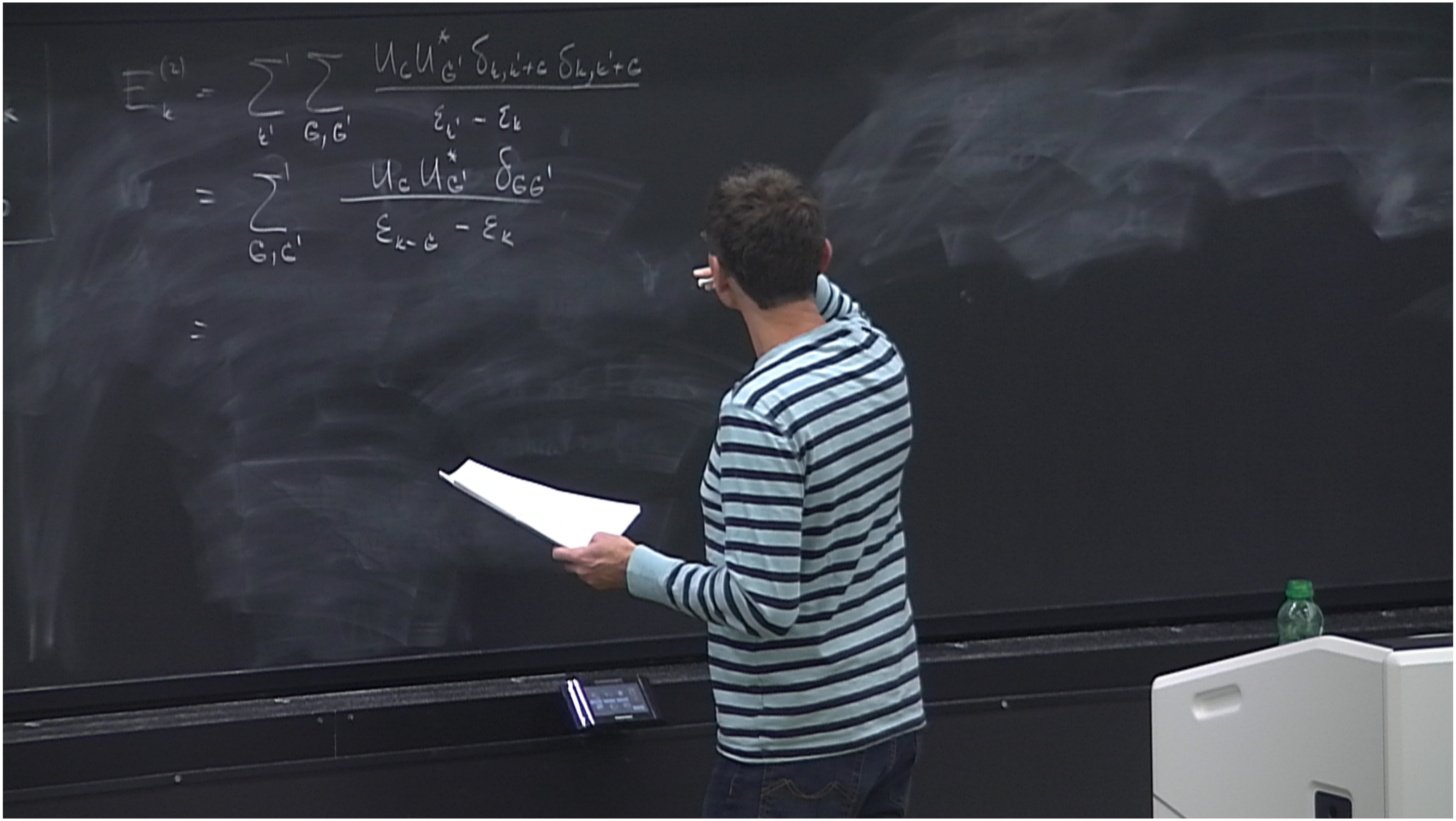
$G = 0$

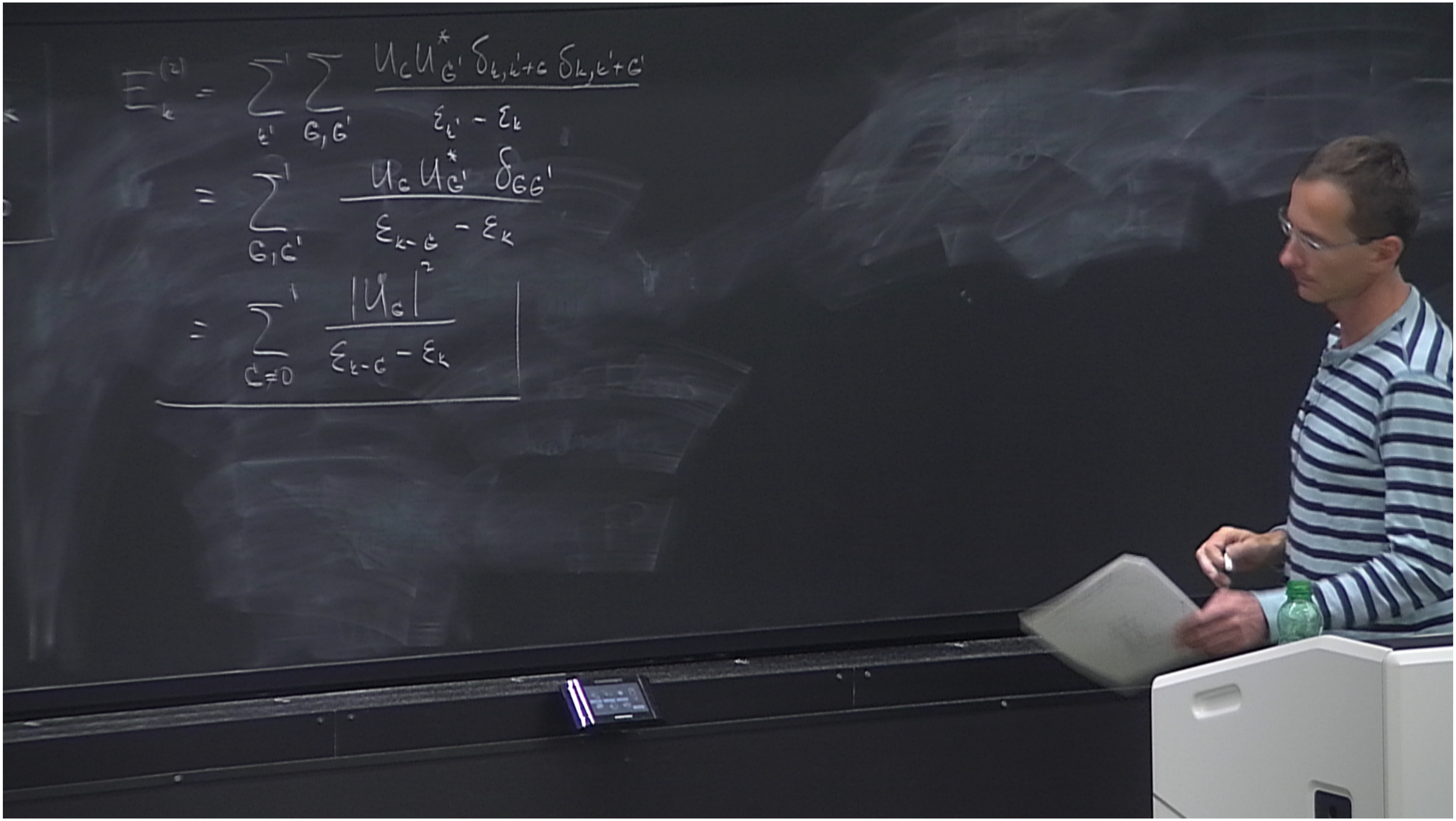
$$E_k^{(2)} = \sum_{k'}{}' \frac{\langle k|H'|k'\rangle\langle k'|H'|k\rangle}{\varepsilon_{k'} - \varepsilon_k}$$

$$\langle k|H'|k'\rangle = \sum_G U_G\, \delta_{k,k'+G}$$

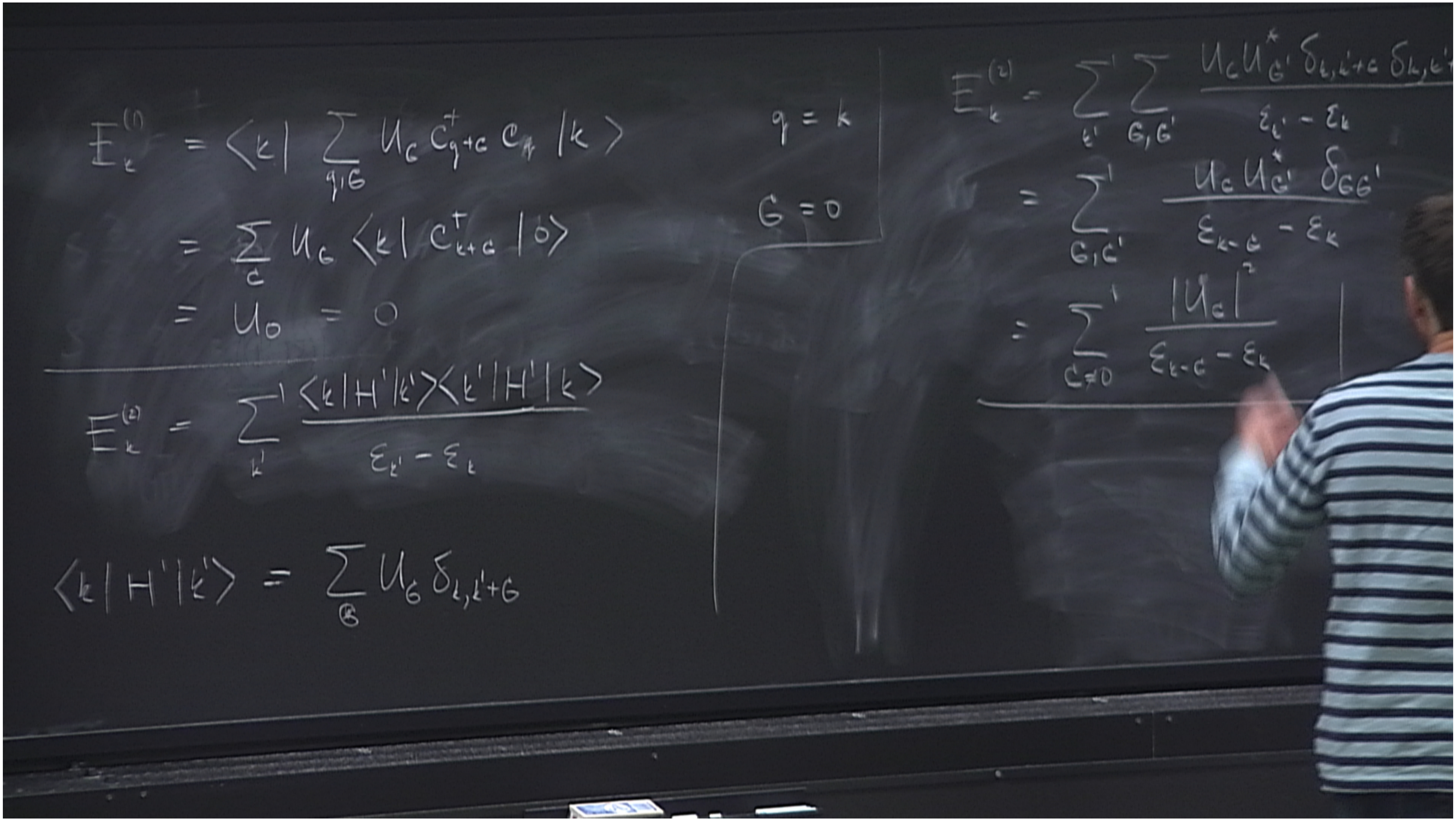
$$E_k^{(2)} = \sum_{k'} \sum_{G,G'}$$

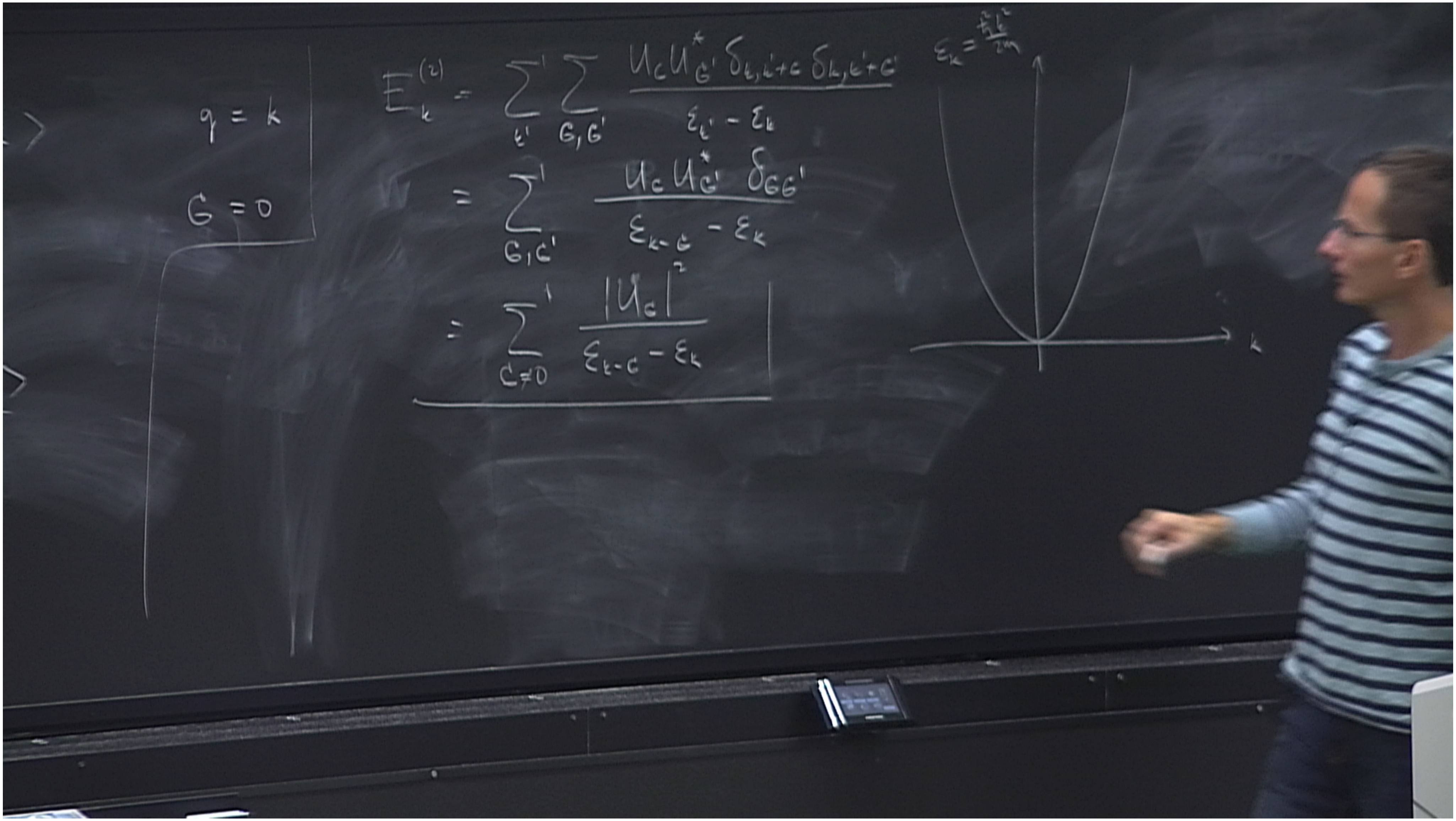

$E_k^{(2)} = \sum_{k'}' \sum_{G,G'} \frac{U_G U_{G'}^{*} \delta_{k,k'+G} \delta_{k,k'+G}}{\varepsilon_{k'} - \varepsilon_k}$


$E_k^{(2)} = \sum_{k'}' \sum_{G,G'} \frac{U_G U_{G'}^* \delta_{k,k'+G} \delta_{k,k'+G'}}{\varepsilon_{k'} - \varepsilon_k}$
$= \sum_{G,G'}' \frac{U_G U_{G'}^* \delta_{GG'}}{\varepsilon_{k-G} - \varepsilon_k}$
$=$

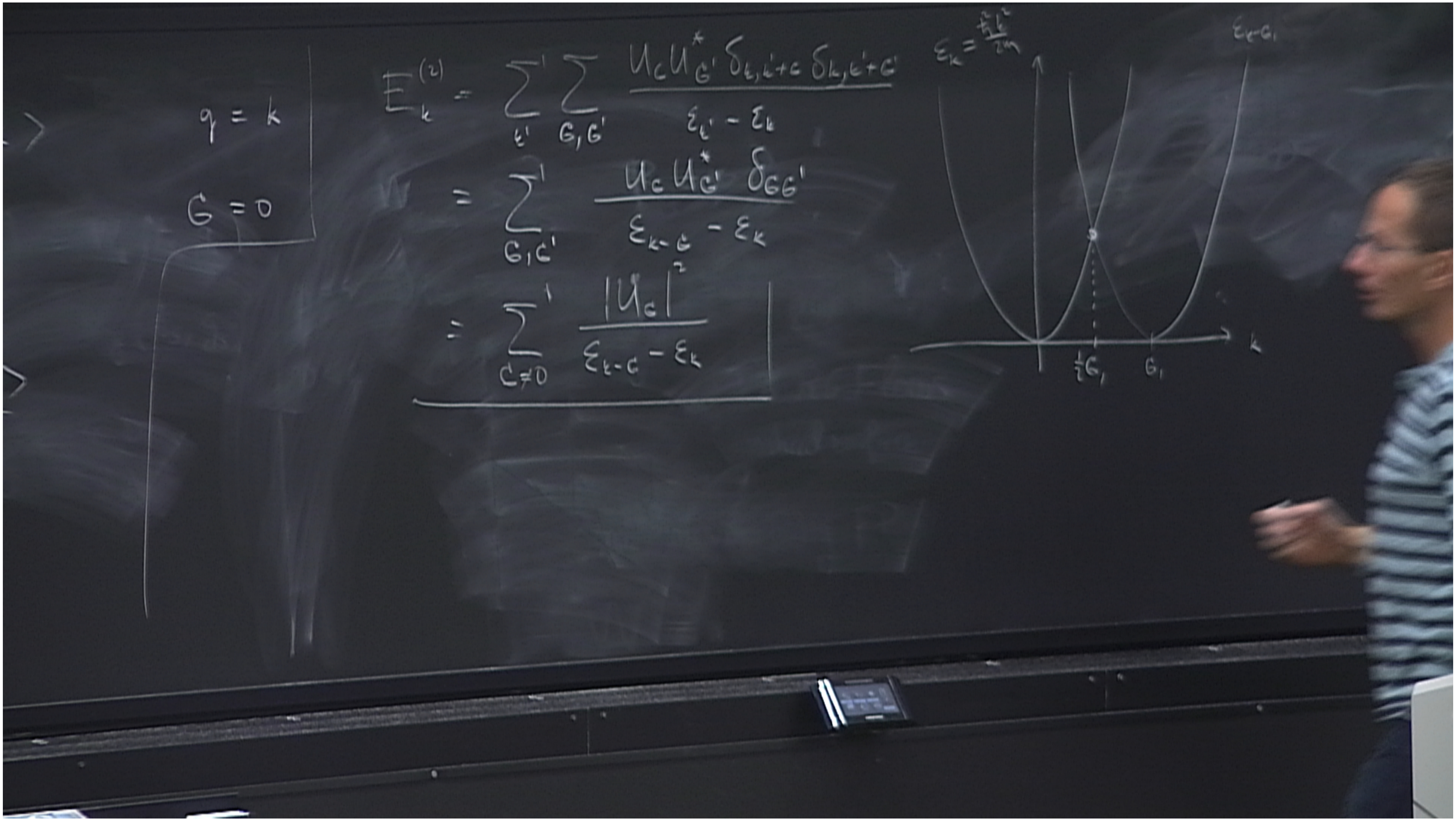


$E_k^{(2)} = \sum_{k'}' \sum_{G,G'} \frac{U_G U_{G'}^* \delta_{k,k'+G} \delta_{k,k'+G'}}{\varepsilon_{k'} - \varepsilon_k}$
$= \sum_{G,G'}' \frac{U_G U_{G'}^* \delta_{GG'}}{\varepsilon_{k-G} - \varepsilon_k}$
$= \sum_{G \neq 0}' \frac{|U_G|^2}{\varepsilon_{k-G} - \varepsilon_k}$

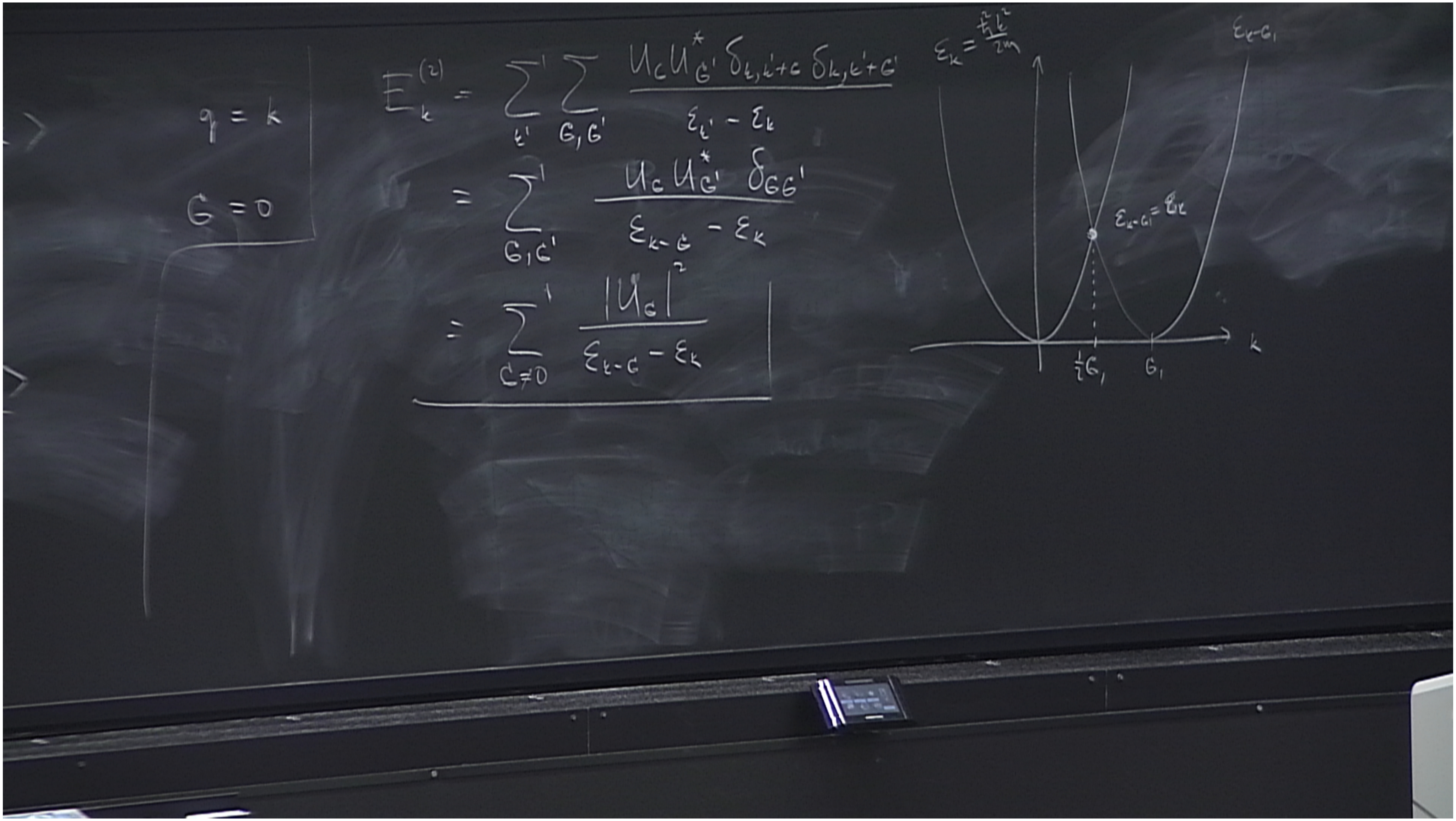

$E_k^{(1)} = \langle k | \sum_{q,G} U_G c^\dagger_{q+G} c_q | k \rangle$
$q = k$
$G = 0$
$= \sum_G U_G \langle k | c^\dagger_{k+G} | 0 \rangle$
$= U_0 = 0$
$E_k^{(2)} = \sum_{k'}' \frac{\langle k|H'|k'\rangle\langle k'|H'|k\rangle}{\varepsilon_{k'} - \varepsilon_k}$
$\langle k | H' | k' \rangle = \sum_G U_G \delta_{k,k'+G}$
$E_k^{(2)} = \sum_{k'}' \sum_{G,G'} \frac{U_G U^*_{G'} \delta_{k,k'+G} \delta_{k,k'+G'}}{\varepsilon_{k'} - \varepsilon_k}$
$= \sum_{G,G'}' \frac{U_G U^*_{G'} \delta_{GG'}}{\varepsilon_{k-G} - \varepsilon_k}$
$= \sum_{G \neq 0}' \frac{|U_G|^2}{\varepsilon_{k-G} - \varepsilon_k}$



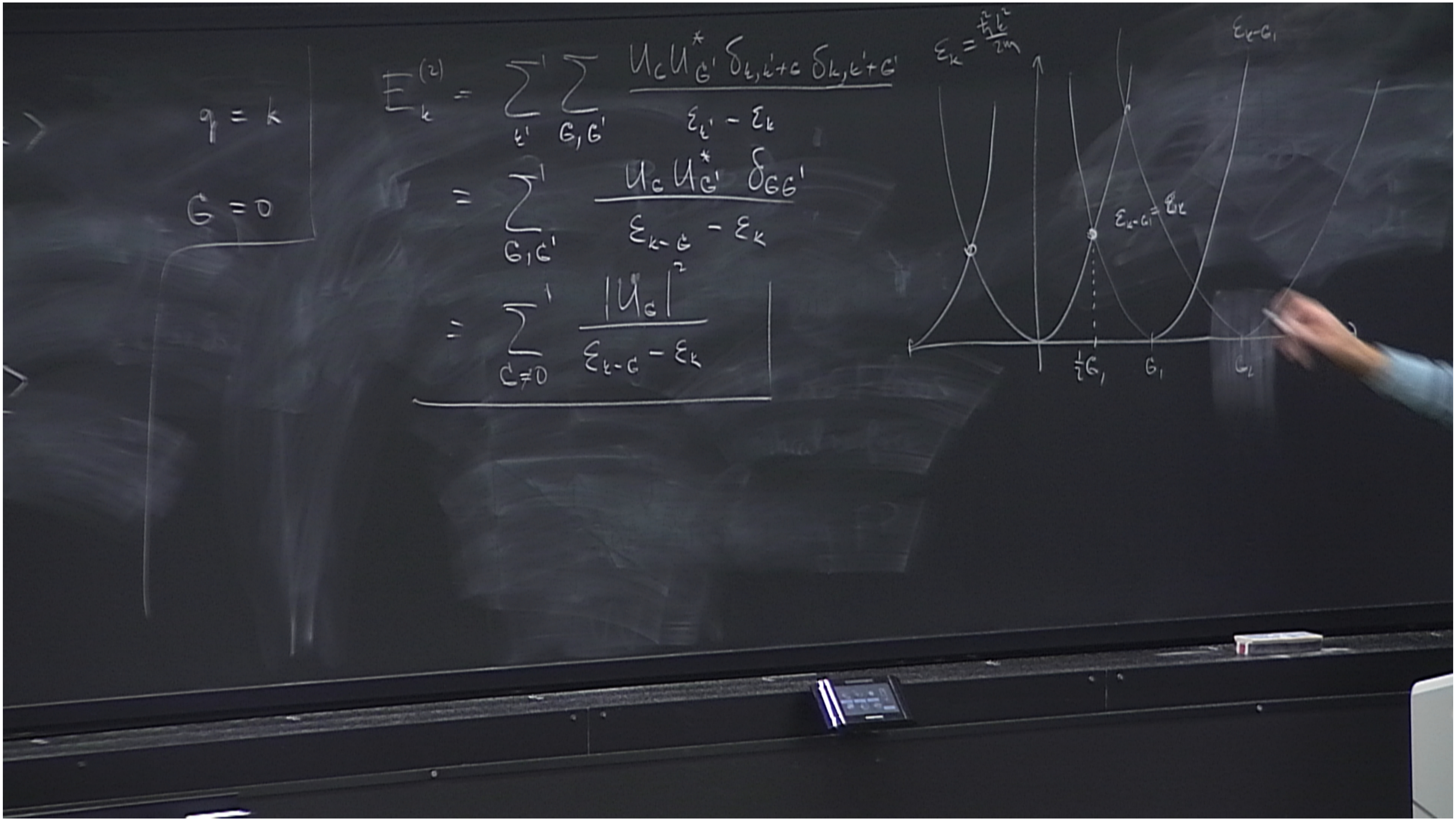
$q = k$
$G = 0$
$E_k^{(2)} = \sum_{k'}' \sum_{G,G'} \frac{U_G U_{G'}^* \delta_{k,k'+G} \delta_{k,k'+G'}}{\varepsilon_{k'} - \varepsilon_k}$
$= \sum_{G,G'}' \frac{U_G U_{G'}^* \delta_{GG'}}{\varepsilon_{k-G} - \varepsilon_k}$
$= \sum_{G \neq 0}' \frac{|U_G|^2}{\varepsilon_{k-G} - \varepsilon_k}$
$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$
k

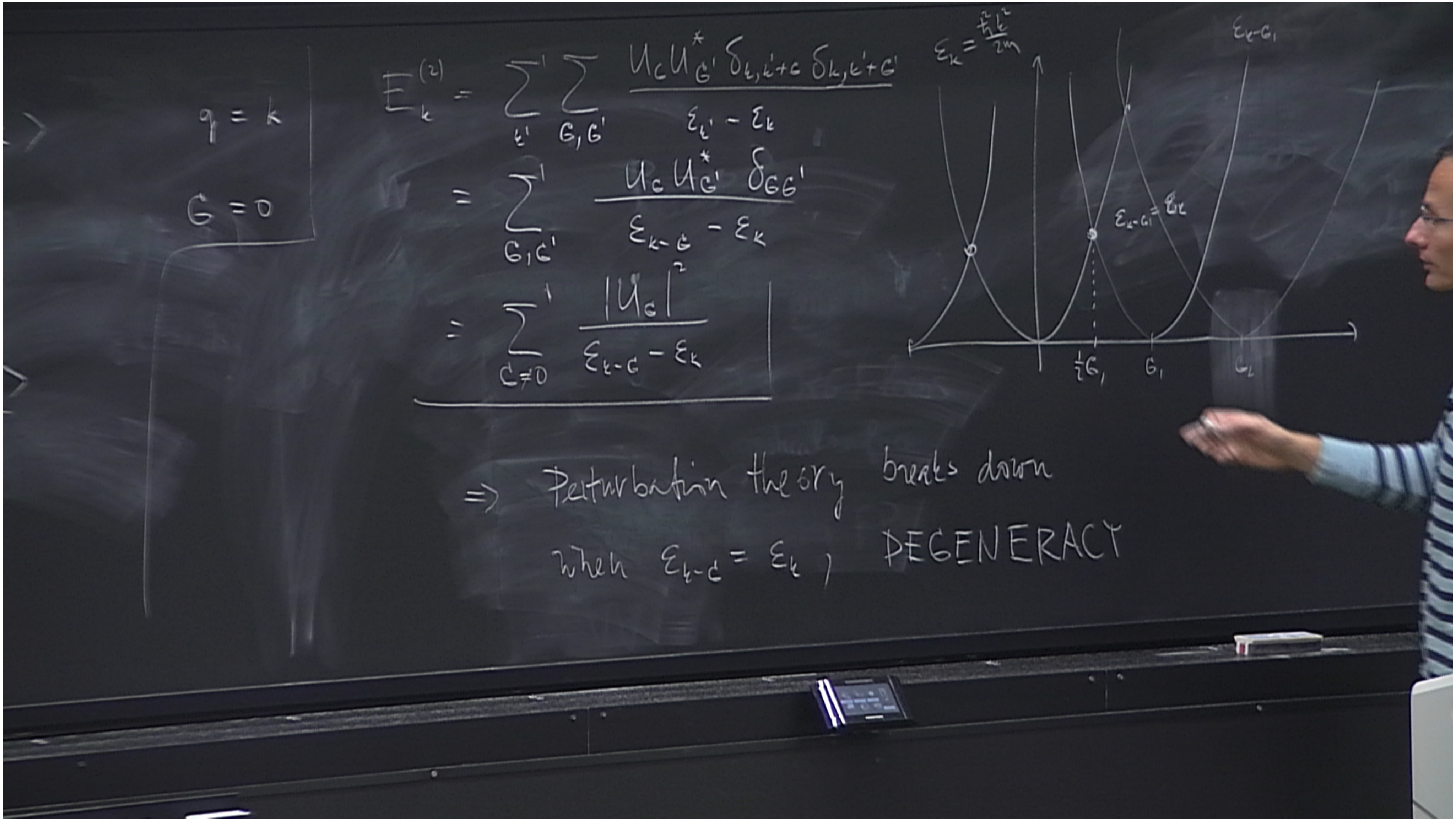


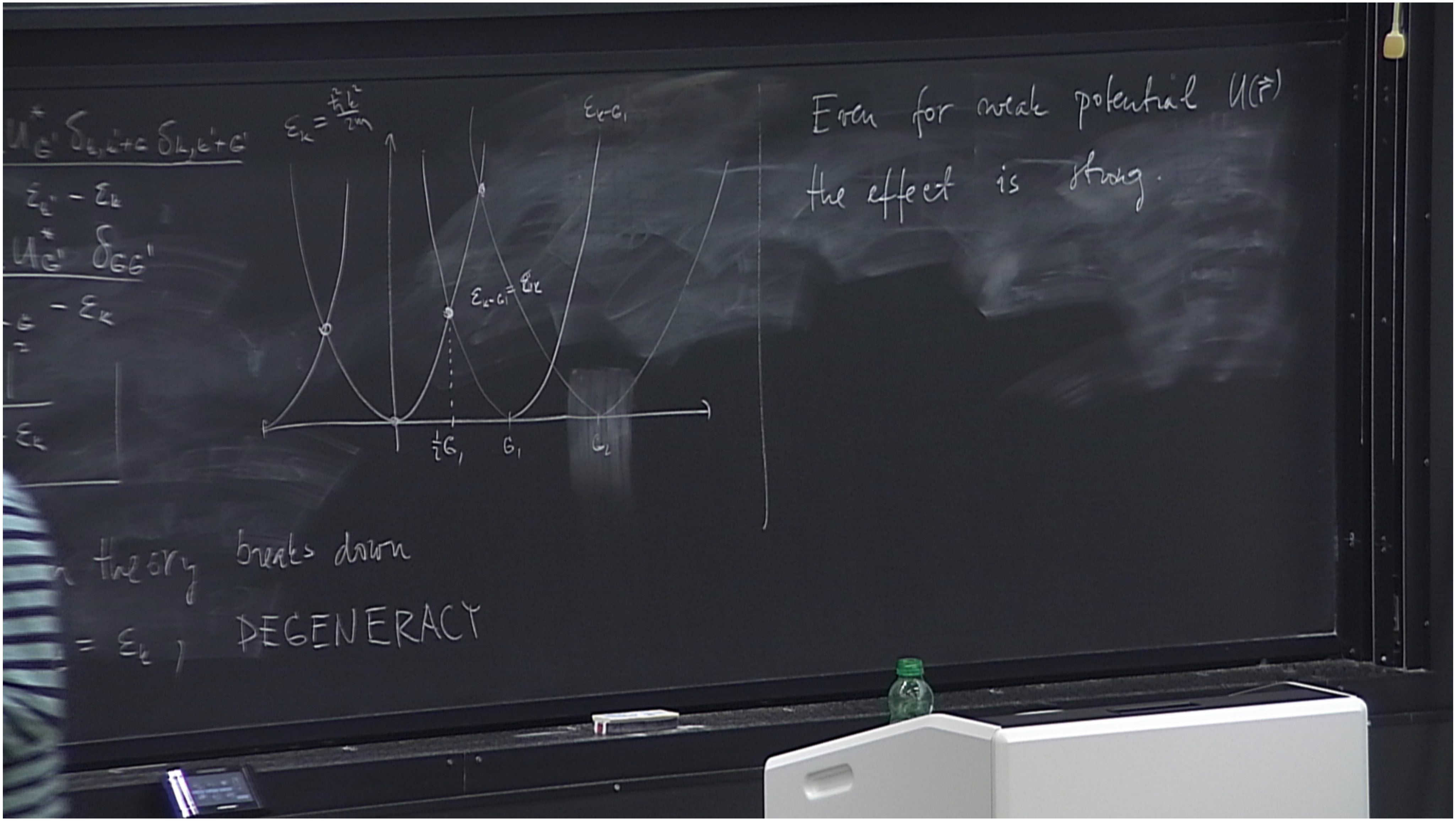
$q = k$
$G = 0$
$E_k^{(2)} = \sum_{k'}' \sum_{G,G'} \frac{U_G U_{G'}^* \delta_{k,k'+G} \delta_{k,k'+G'}}{\varepsilon_{k'} - \varepsilon_k}$
$= \sum_{G,G'}' \frac{U_G U_{G'}^* \delta_{GG'}}{\varepsilon_{k-G} - \varepsilon_k}$
$= \sum_{G\neq 0}' \frac{|U_G|^2}{\varepsilon_{k-G} - \varepsilon_k}$
$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$
ε_{k-G_1}
k
$\frac{1}{2}G_1$
G_1



$q = k$
$G = 0$
$E_k^{(2)} = \sum_{k'}' \sum_{G,G'} \frac{U_G U_{G'}^* \delta_{k,k'+G} \delta_{k,k'+G'}}{\varepsilon_{k'} - \varepsilon_k}$
$= \sum_{G,G'}' \frac{U_G U_{G'}^* \delta_{GG'}}{\varepsilon_{k-G} - \varepsilon_k}$
$= \sum_{G \neq 0}' \frac{|U_G|^2}{\varepsilon_{k-G} - \varepsilon_k}$
$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$
ε_{k-G_1}
$\varepsilon_{k-G_1} = \varepsilon_k$
k
$\frac{1}{2}G_1$
G_1

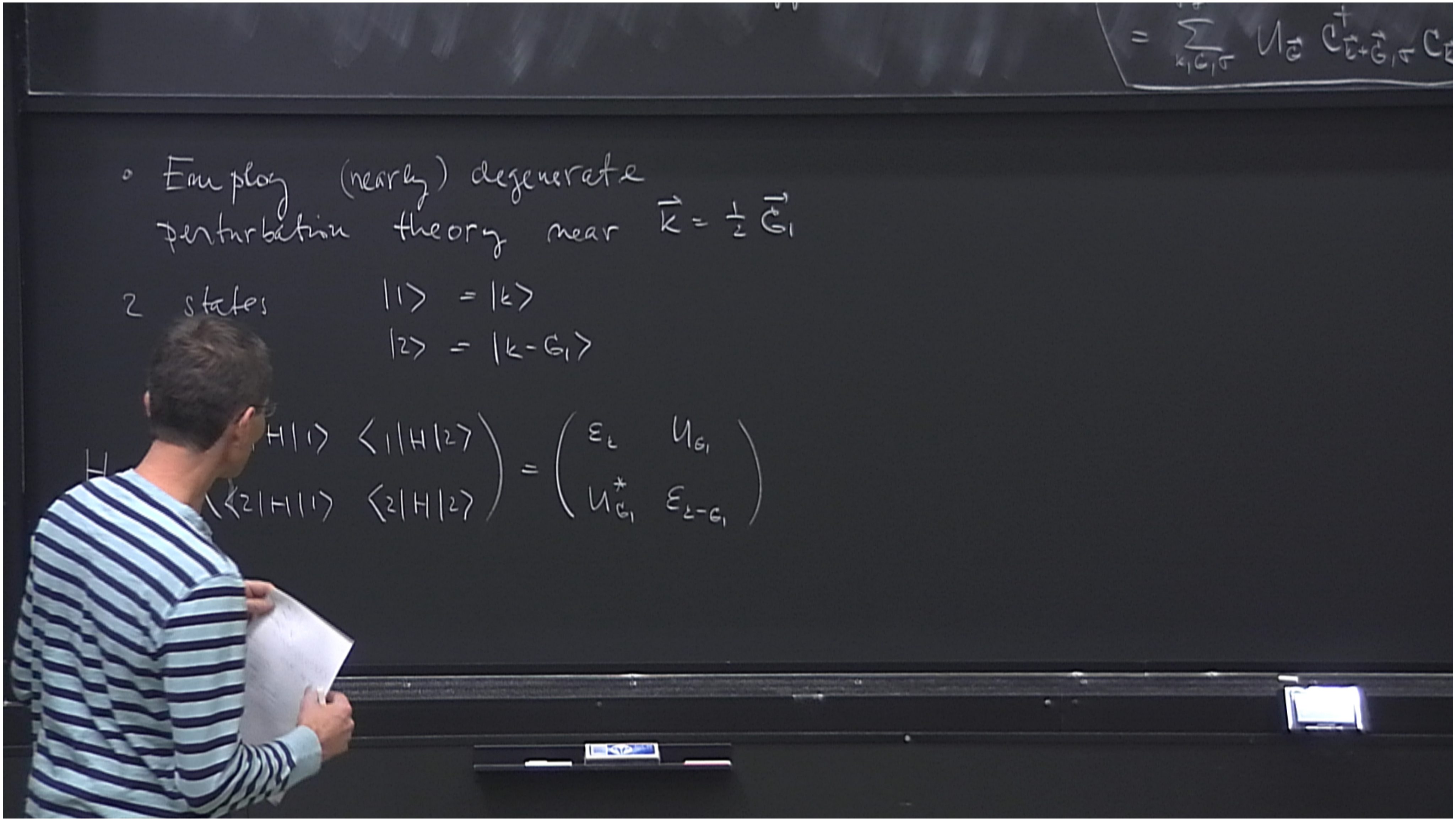

q = k
G = 0
$E_k^{(2)} = \sum_{k'}' \sum_{G,G'} \frac{U_G U_{G'}^* \delta_{k,k'+G} \delta_{k,k'+G'}}{\varepsilon_{k'} - \varepsilon_k}$
$= \sum_{G,G'}' \frac{U_G U_{G'}^* \delta_{GG'}}{\varepsilon_{k-G} - \varepsilon_k}$
$= \sum_{G \neq 0}' \frac{|U_G|^2}{\varepsilon_{k-G} - \varepsilon_k}$
$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$
ε_{k-G_1}
$\varepsilon_{k-G_1} = \varepsilon_k$
$\frac{1}{2}G_1$
G_1
G_2

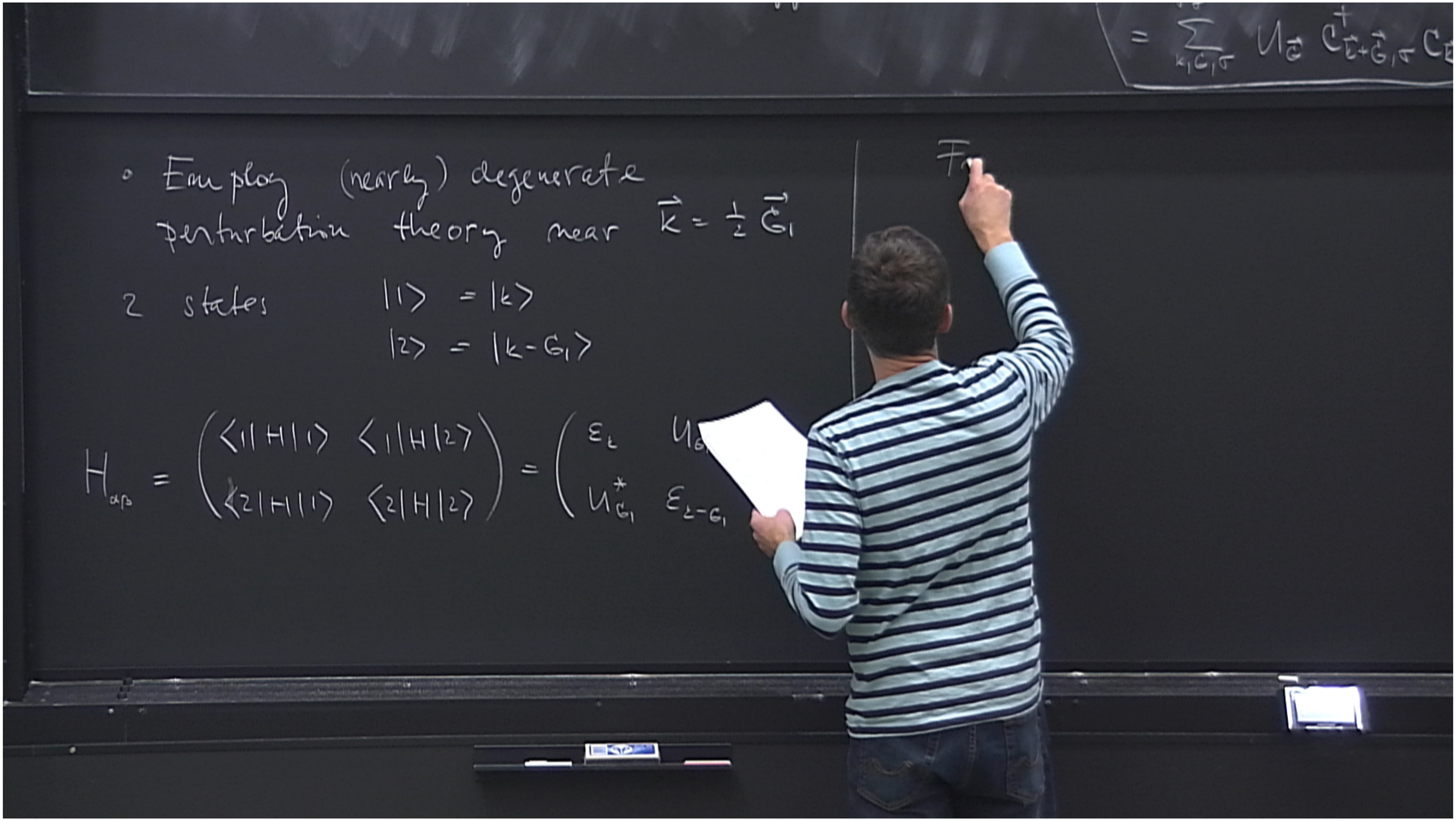

q = k
G = 0
$E_k^{(2)} = \sum_{k'}' \sum_{G,G'} \frac{U_G U_{G'}^* \delta_{k,k'+G} \delta_{k,k'+G'}}{\epsilon_{k'} - \epsilon_k}$
$= \sum_{G,G'}' \frac{U_G U_{G'}^* \delta_{GG'}}{\epsilon_{k-G} - \epsilon_k}$
$= \sum_{G \neq 0}' \frac{|U_G|^2}{\epsilon_{k-G} - \epsilon_k}$
$\epsilon_k = \frac{\hbar^2 k^2}{2m}$
ϵ_{k-G_1}
$\epsilon_{k-G_1} = \epsilon_k$
$\frac{1}{2}G_1$
G_1
G_2
$\Rightarrow$ Perturbation theory breaks down
when $\epsilon_{k-G} = \epsilon_k$, DEGENERACY


Even for weak potential U(r⃗)
the effect is strong.
theory breaks down
DEGENERACY

$= \sum_{k,G,\sigma} U_{\vec{G}}\, c^\dagger_{\vec{k}+\vec{G},\sigma} c_{\vec{k}}$

- Employ (nearly) degenerate perturbation theory near $\vec{k} = \frac{1}{2}\vec{G}_1$


$= \sum_{k, G, \sigma} U_{\vec{G}} \, c^\dagger_{\vec{k}+\vec{G}, \sigma} c_{\vec{k}}$
∘ Employ (nearly) degenerate
perturbation theory near $\vec{k} = \frac{1}{2}\vec{G}_1$
2 states $|1\rangle = |k\rangle$
$|2\rangle = |k - G_1\rangle$
$H|1\rangle$ $\langle 1|H|2\rangle$
$\langle 2|H|1\rangle$ $\langle 2|H|2\rangle$
$= \begin{pmatrix} \varepsilon_k & U_{G_1} \\ U^*_{G_1} & \varepsilon_{k-G_1} \end{pmatrix}$


$= \sum_{k,G,\sigma} U_{\vec{G}} c^\dagger_{\vec{k}+\vec{G},\sigma} c_{\vec{k}}$
∘ Employ (nearly) degenerate perturbation theory near $\vec{k} = \frac{1}{2}\vec{G}_1$
2 states $|1\rangle = |k\rangle$
$|2\rangle = |k-G_1\rangle$
$H_{\alpha\beta} = \begin{pmatrix} \langle 1|H|1\rangle & \langle 1|H|2\rangle \\ \langle 2|H|1\rangle & \langle 2|H|2\rangle \end{pmatrix} = \begin{pmatrix} \varepsilon_k & U_{G_1} \\ U^*_{G_1} & \varepsilon_{k-G_1} \end{pmatrix}$

$$= \sum_{k,G,\sigma} U_{\vec{G}}\, c^{\dagger}_{\vec{k}+\vec{G},\sigma} c_{\vec{k}\sigma}$$

Find energy eigenvalues of H_{aro}

$$\begin{vmatrix} \varepsilon_k - E & U_G \\ U_G^* & \varepsilon_{k-G} - E \end{vmatrix} = 0$$

$$E = \frac{1}{2}(\varepsilon_k + \varepsilon_{k-G}) \pm \sqrt{\frac{1}{4}(\varepsilon_k - \varepsilon_{k-G})^2 + |U_G|^2}$$

$$= \sum_{k,G,\sigma} U_{\vec{G}}\, c^{\dagger}_{\vec{k}+\vec{G},\sigma} c_{\vec{k}\sigma}$$

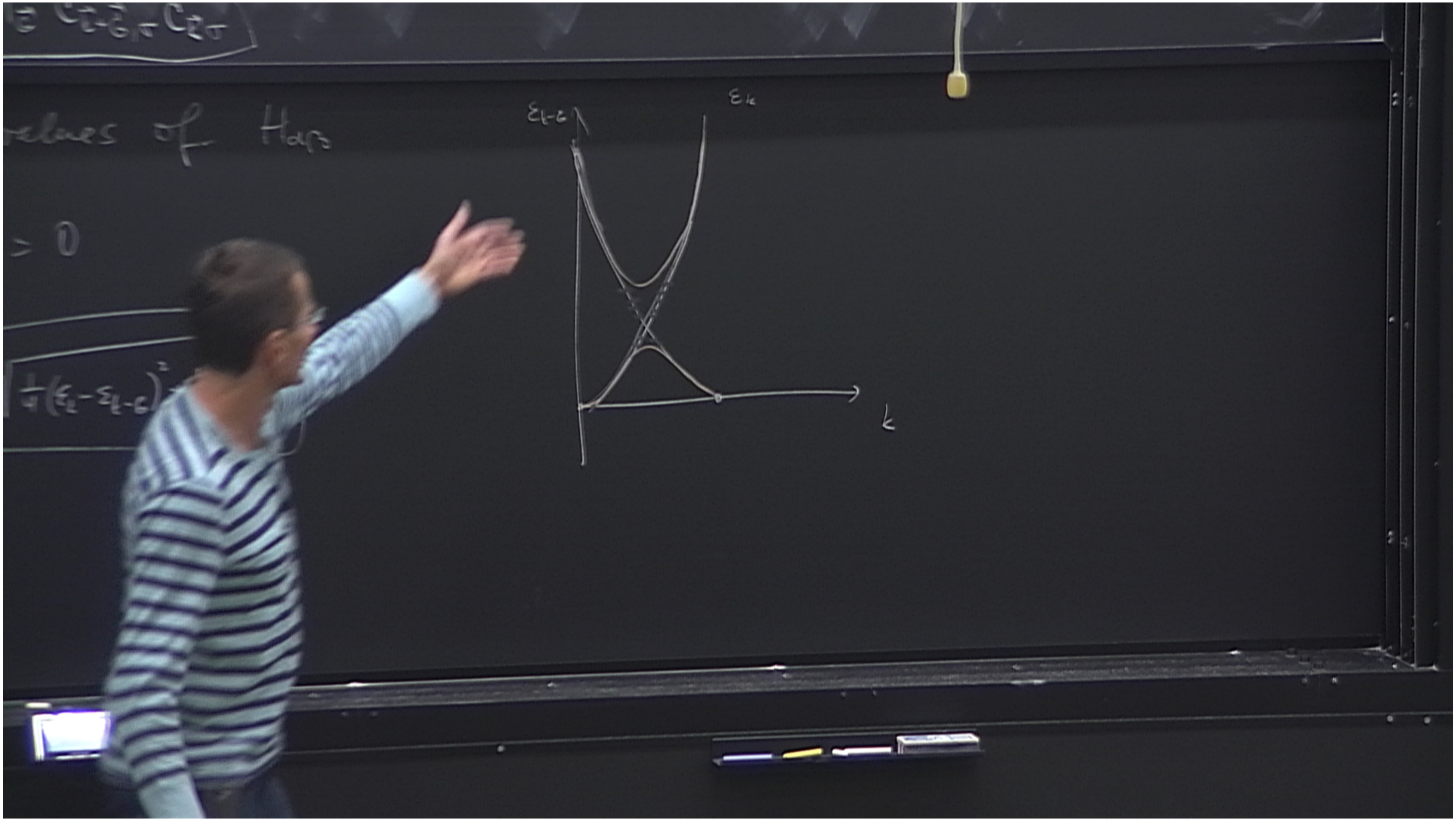
Find energy eigenvalues of H_{MF}

$$\begin{vmatrix} \varepsilon_k - E & U_G \\ U_G^* & \varepsilon_{k-G} - E \end{vmatrix} = 0$$

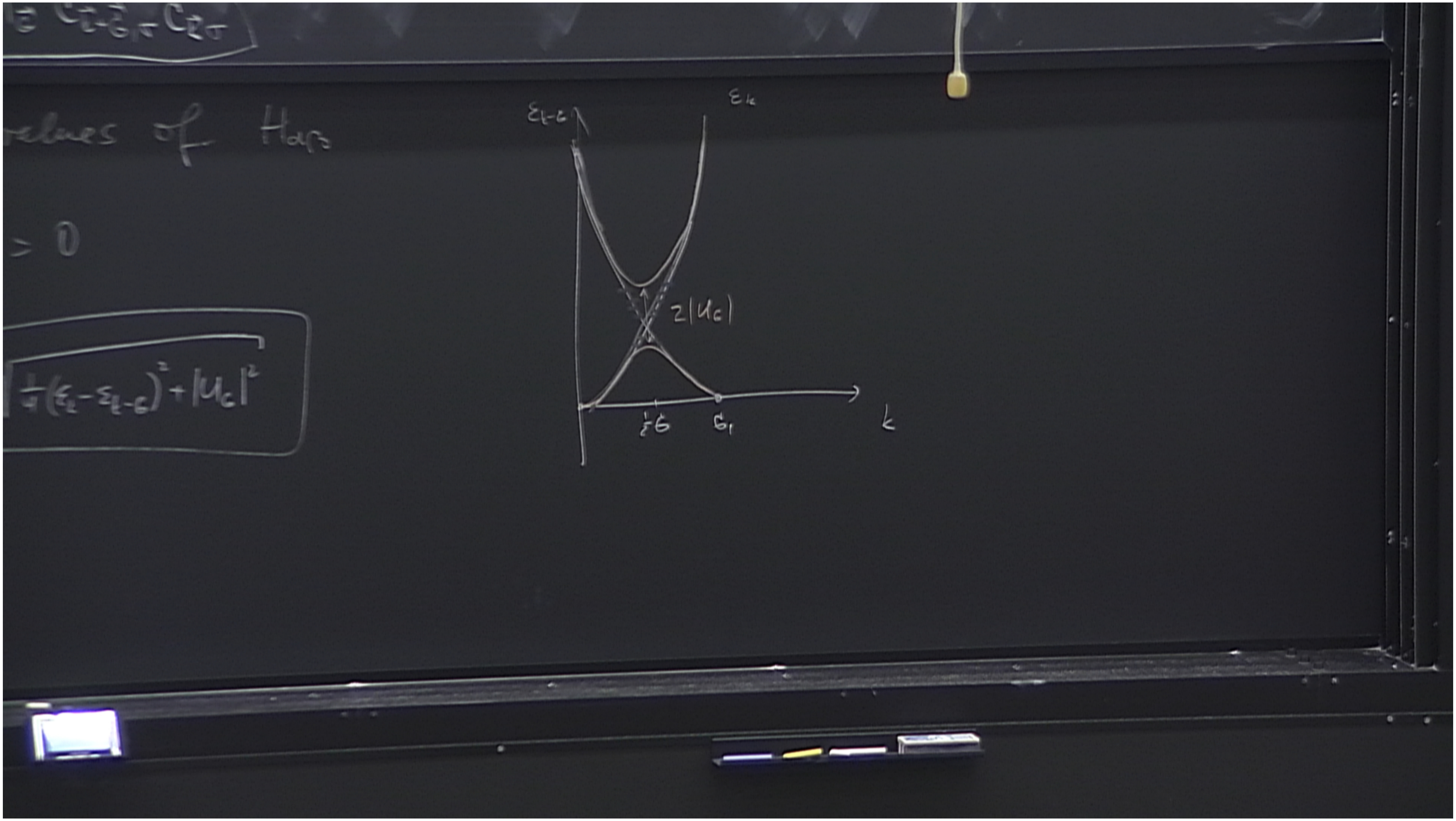
$$\boxed{E = \frac{1}{2}(\varepsilon_k + \varepsilon_{k-G}) \pm \sqrt{\frac{1}{4}(\varepsilon_k - \varepsilon_{k-G})^2 + |U_G|^2}}$$

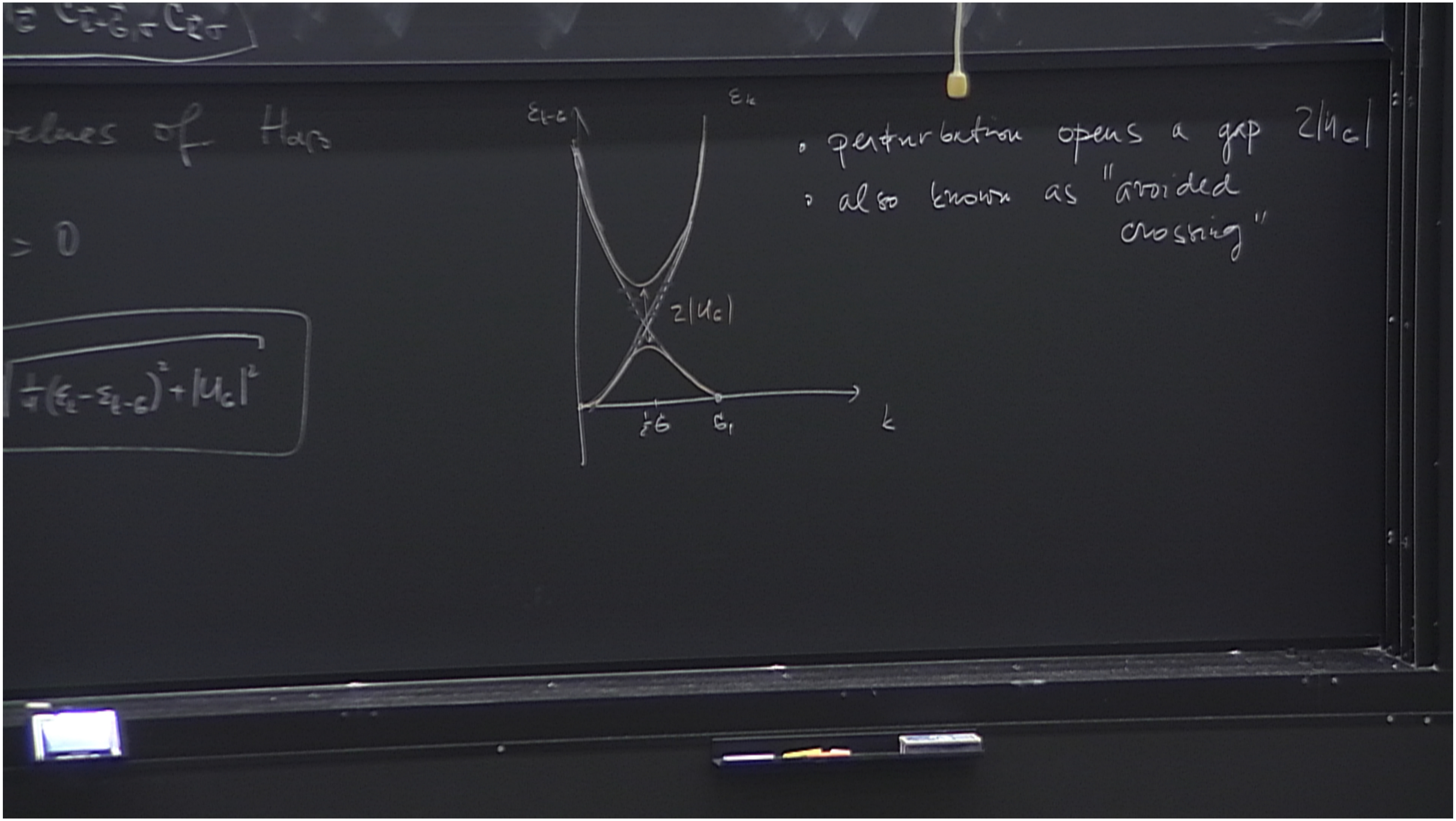
For $\vec{k} = \frac{1}{2}\vec{G}$

$$E_k = \varepsilon_k \pm |U_G|$$

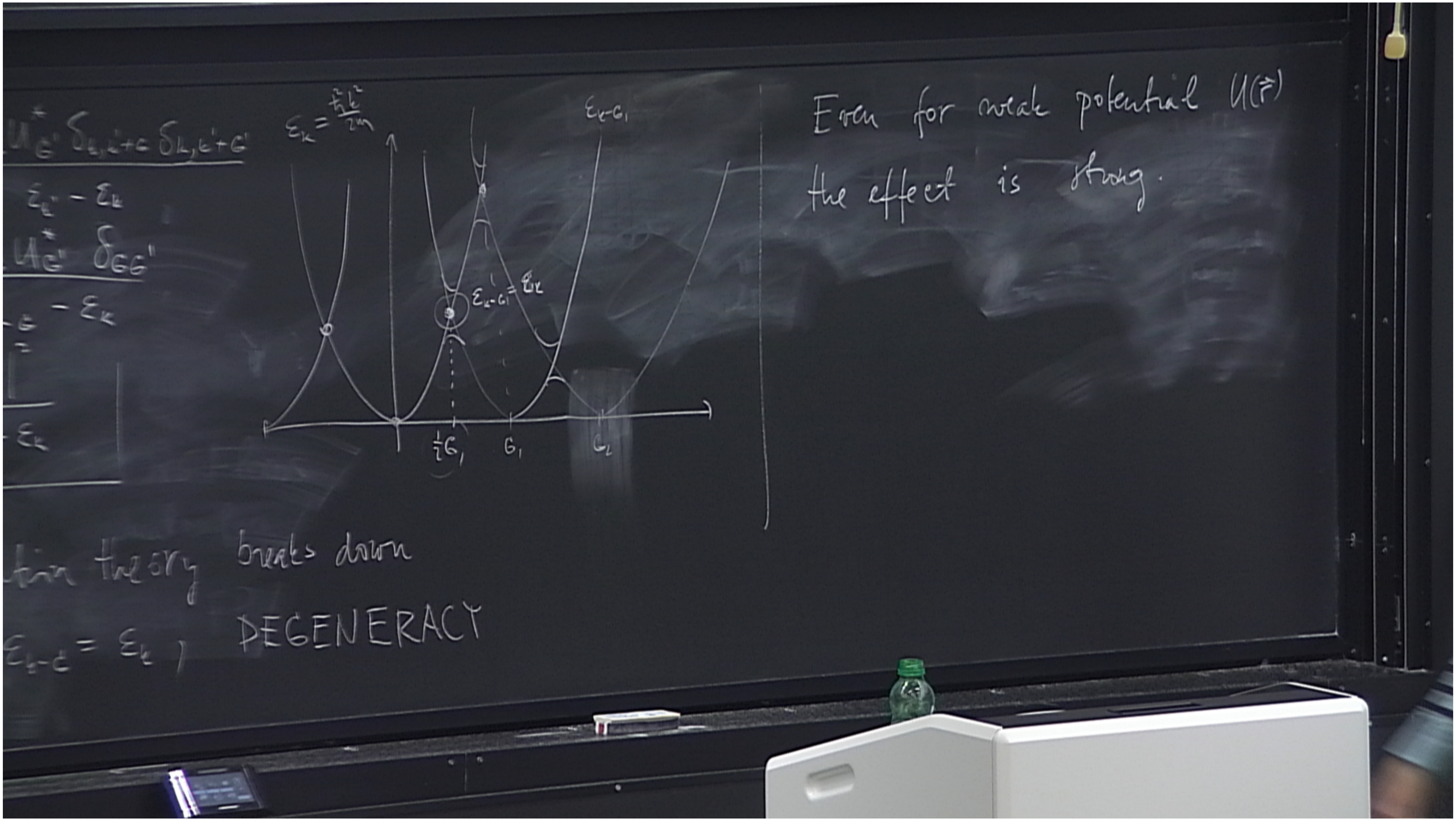


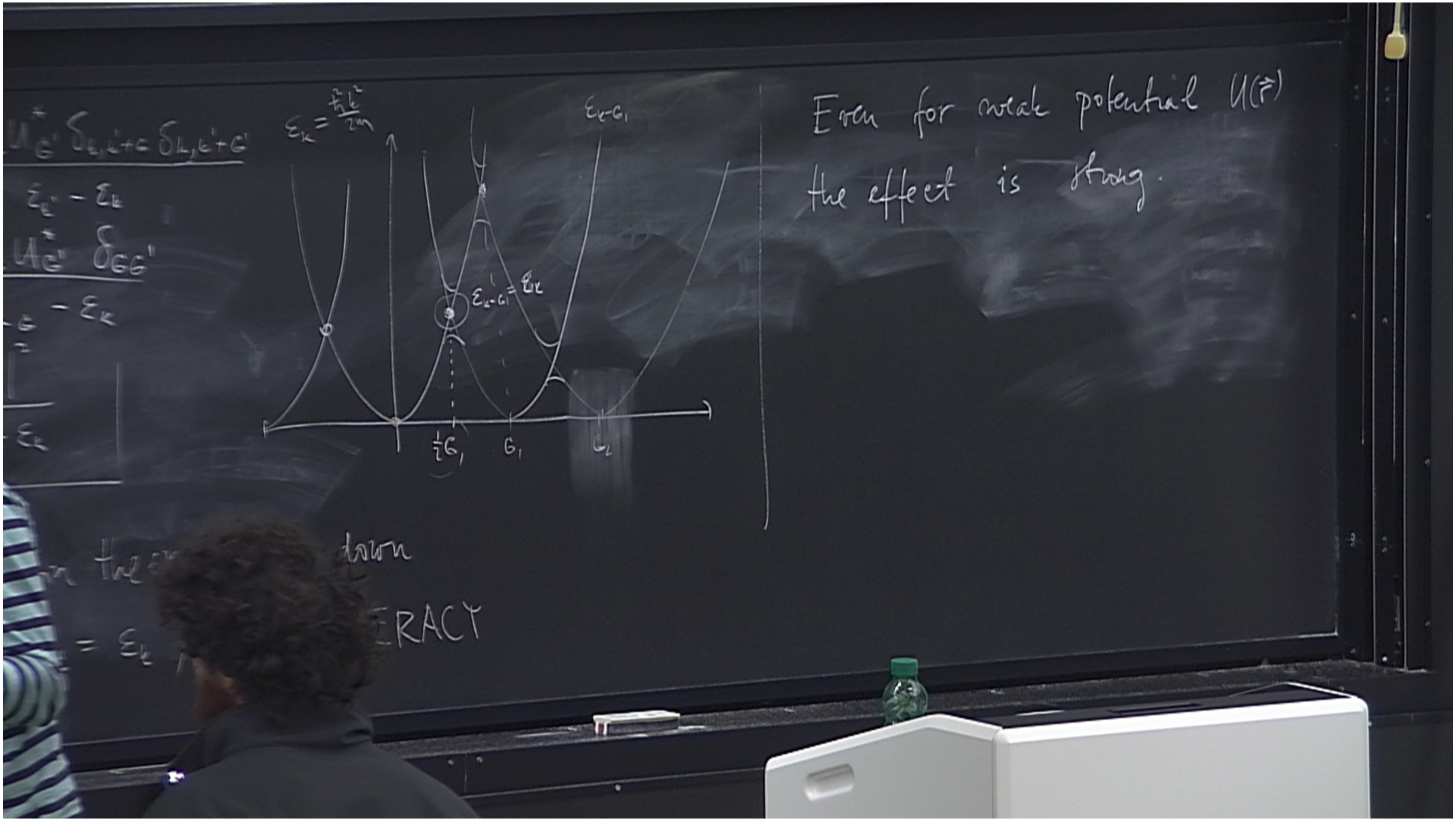
k


values of H
> 0
$\sqrt{\frac{1}{4}(\varepsilon_k - \varepsilon_{k-G})^2 + |U_G|^2}$
ε_{k-G}
ε_k
$2|U_G|$
$\frac{1}{2}G$
k



ε_{k-G}
ε_k
$2|U_G|$
$\frac{1}{2}G$
G_1
k
$\frac{1}{4}(\varepsilon_k-\varepsilon_{k-G})^2+|U_G|^2$
∘ perturbation opens a gap $2|U_G|$
∘ also known as "avoided crossing"


Even for weak potential U(r)
the effect is strong.
theory breaks down
DEGENERACY
ε_{k-G1} = ε_k
G1
G2


Even for weak potential U(r)
the effect is strong.
down
ERACY