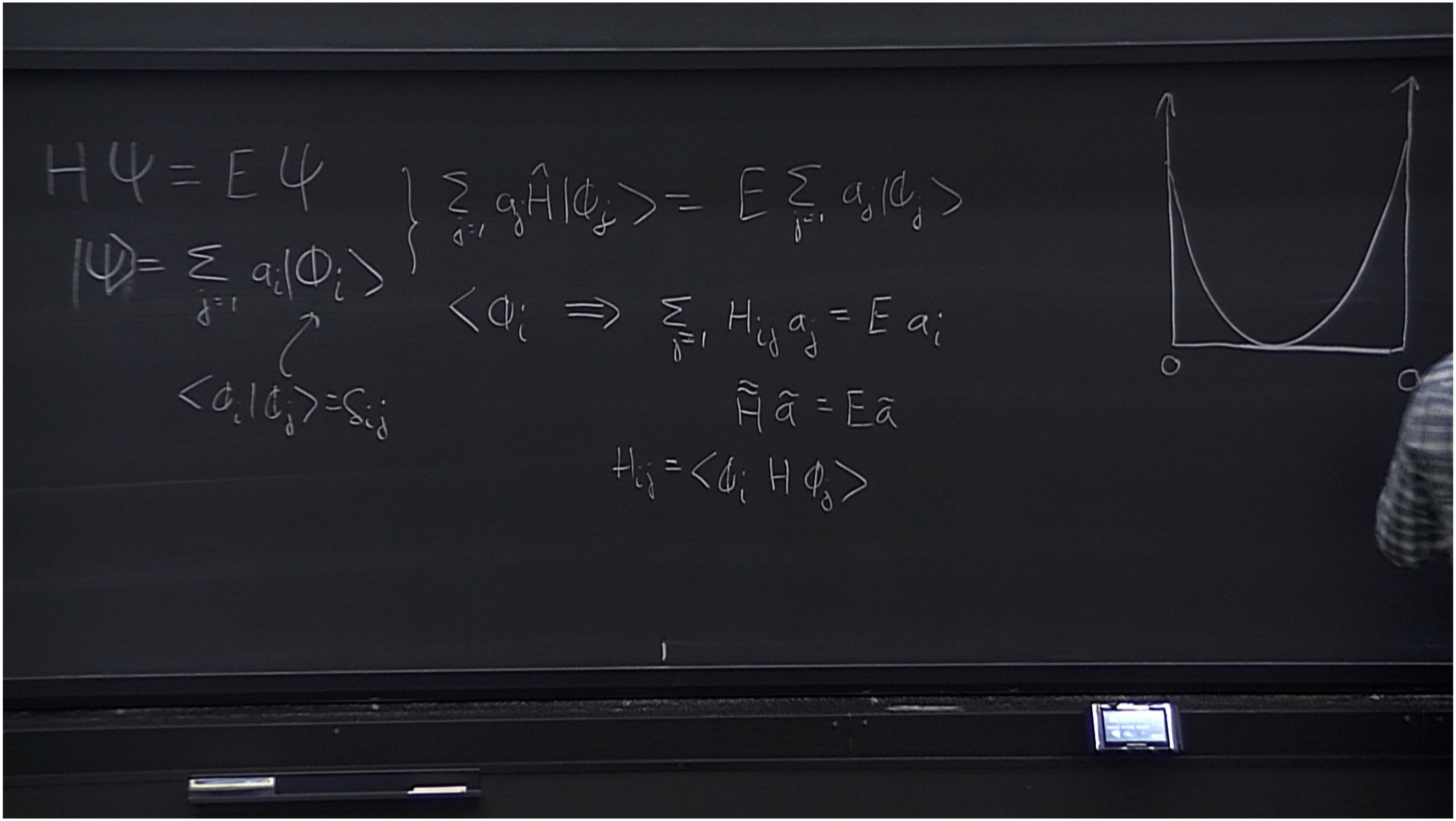
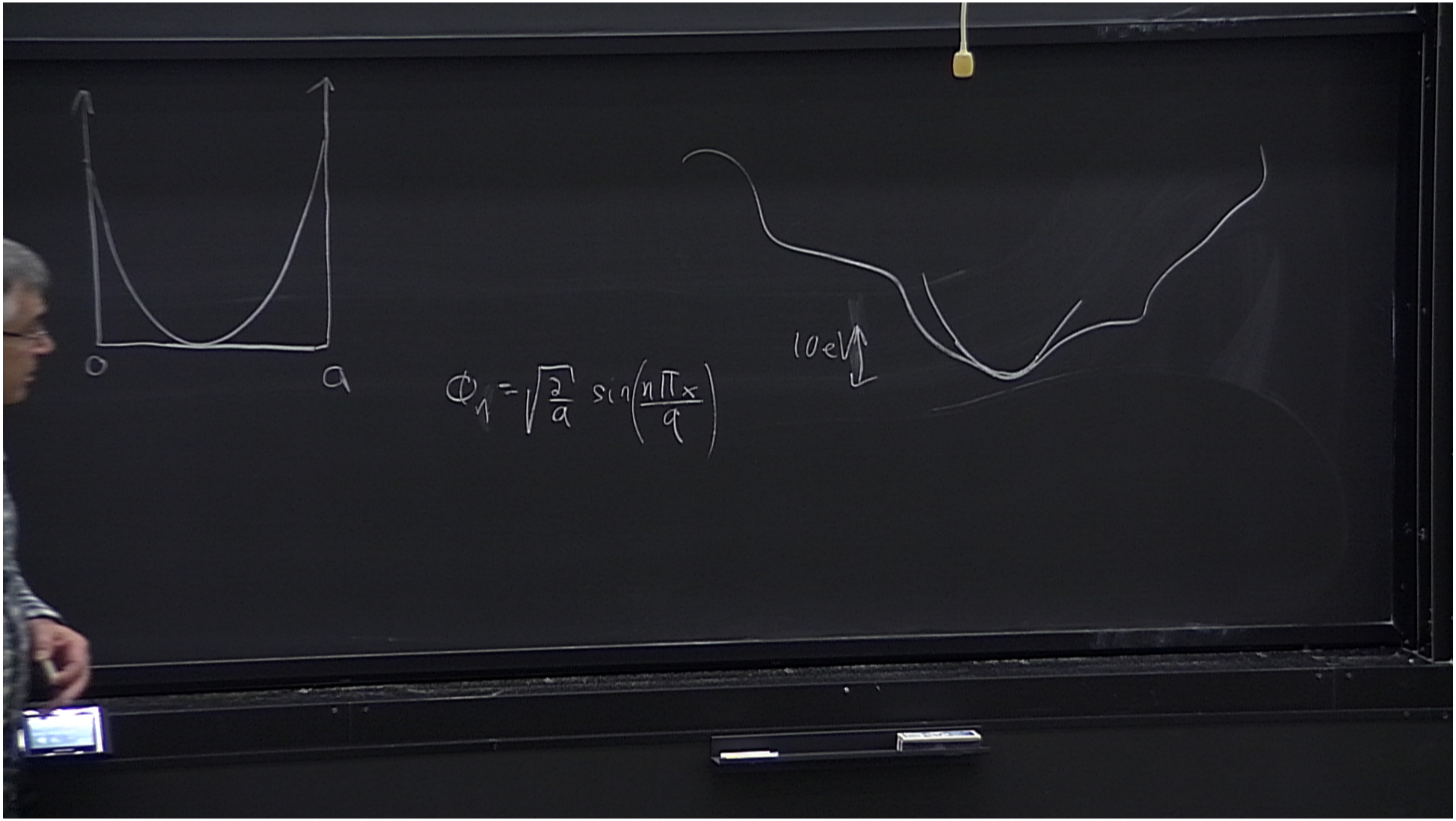
Title: PSI 2016/2017 Condensed Matter - Lecture 3

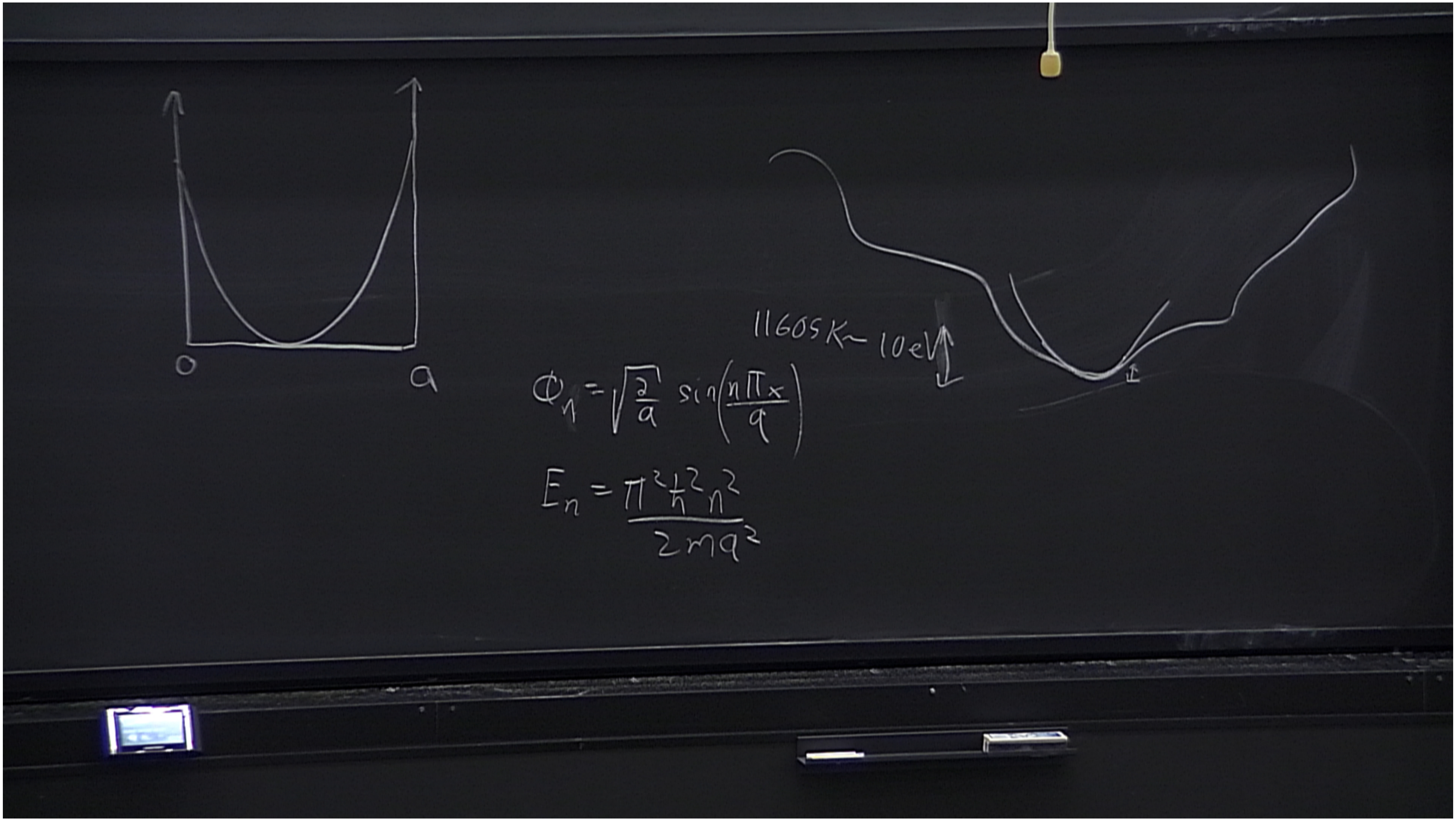
Date: Nov 09, 2016 10:45 AM

URL: http://pirsa.org/16110054

Abstract:


$H\psi = E\psi$
$|\psi\rangle = \sum_{j=1} a_i |\Phi_i\rangle$
$\langle \phi_i | \phi_j \rangle = \delta_{ij}$
$\sum_{j=1} a_j \hat{H} |\phi_j\rangle = E \sum_{j=1} a_j |\phi_j\rangle$
$\langle \phi_i \Longrightarrow \sum_{j=1} H_{ij} a_j = E a_i$
$\tilde{H} \tilde{a} = E \tilde{a}$
$H_{ij} = \langle \phi_i H \phi_j \rangle$
0
0


0
a
$\Phi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$
10eV


0
a
11605 K ~ 10 eV
$\Phi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$
$E_n = \frac{\pi^2 \hbar^2 n^2}{2ma^2}$

Perimeter: Condensed Matter   Fall 2016

…Metals, Insulators, Magnets, and Superconductors…

supplementary material to Lecture 3, etc.

F. Marsiglio

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The harmonic oscillator in quantum mechanics: A third way

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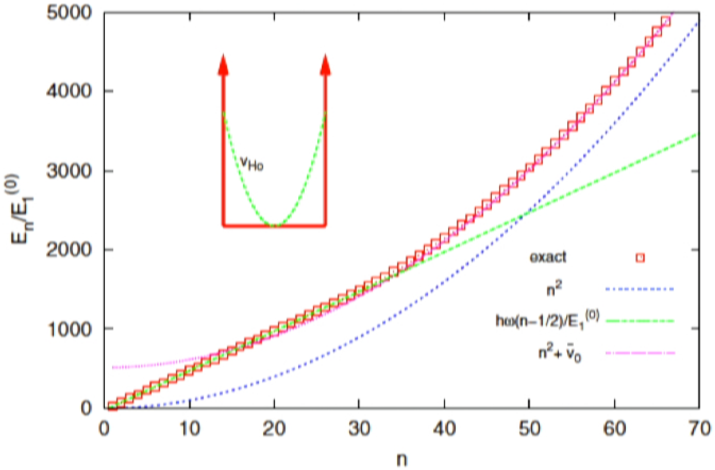
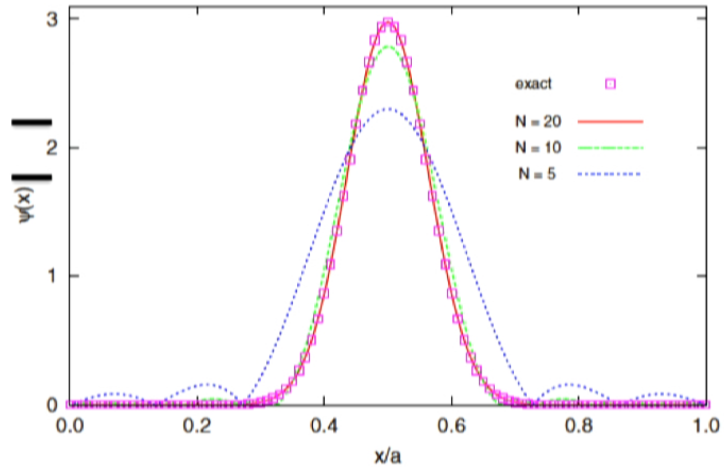
253 Am. J. Phys. 77 (3), March 2009





$$h_{nm} \equiv H_{nm}/E_1^{(0)} = \delta_{nm}\left[n^2 + \frac{\pi^2}{48}\left(\frac{\hbar\omega}{E_1^{(0)}}\right)^2\left(1 - \frac{6}{(\pi n)^2}\right)\right] + (1-\delta_{nm})\left(\frac{\hbar\omega}{E_1^{(0)}}\right)^2 g_{nm}, \qquad (11)$$

where

$$g_{nm} = \left(\frac{(-1)^{n+m}+1}{4}\right)\left(\frac{1}{(n-m)^2} - \frac{1}{(n+m)^2}\right). \qquad (12)$$

The Kronig-Penney model extended to arbitrary potentials via numerical matrix mechanics

R. L. Pavelich and F. Marsiglio

Citation: American Journal of Physics **83**, 773 (2015); doi: 10.1119/1.4923026
View online: http://dx.doi.org/10.1119/1.4923026

B. Square well with periodic boundary conditions

$$\phi(x+a) = \phi(x),$$

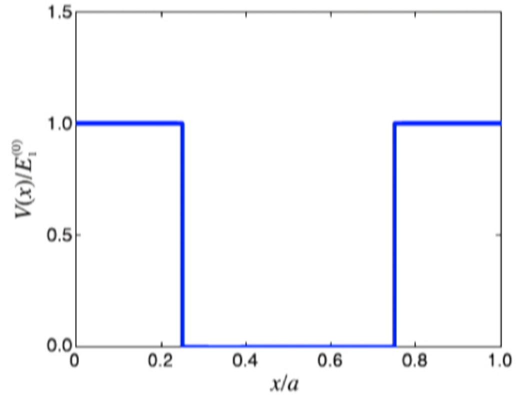


Fig. 3. Central square well with $v_0 = 1$ and $\rho = 0.5$.

777 Am. J. Phys., Vol. 83, No. 9, September 2015

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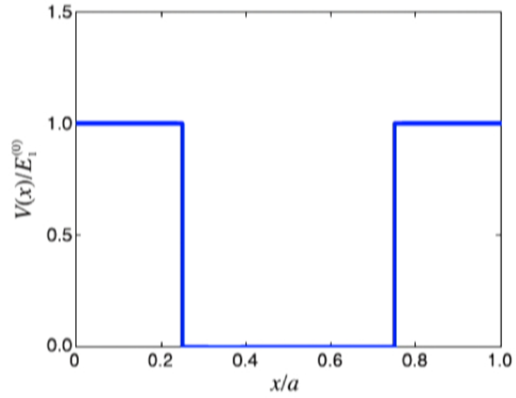

Fig. 3. Central square well with $v_0 = 1$ and $\rho = 0.5$.

777 Am. J. Phys., Vol. 83, No. 9, September 2015

B. Square well with periodic boundary conditions

$$\phi(x+a) = \phi(x),$$

A. Bloch's theorem

$$\psi(x+a) = e^{iKa}\psi(x),$$

K = k

$$h_{nm} = \delta_{nm}\left[\left(2n + \frac{Ka}{\pi}\right)^2 + v_0(1-\rho)\right] + (1-\delta_{nm})v_0\frac{(-1)^{m-n+1}}{\pi}\frac{\sin[\pi(m-n)\rho]}{m-n}. \qquad (28)$$

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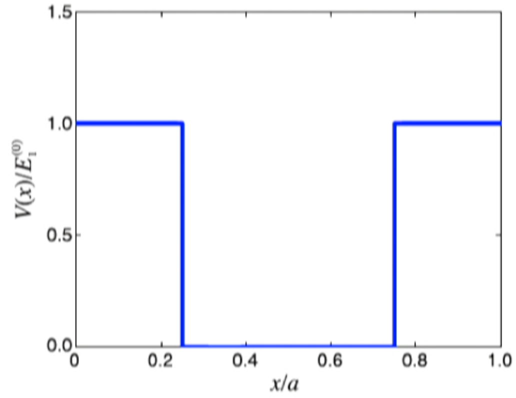

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$$h_{nm} = \begin{pmatrix} (0+Ka/\pi)^2 + h^V_{00} & h^V_{01} & h^V_{02} & \cdots \\ h^V_{10} & (2+Ka/\pi)^2 + h^V_{11} & h^V_{12} & \cdots \\ h^V_{20} & h_{21} & (4+Ka/\pi)^2 + h^V_{22} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

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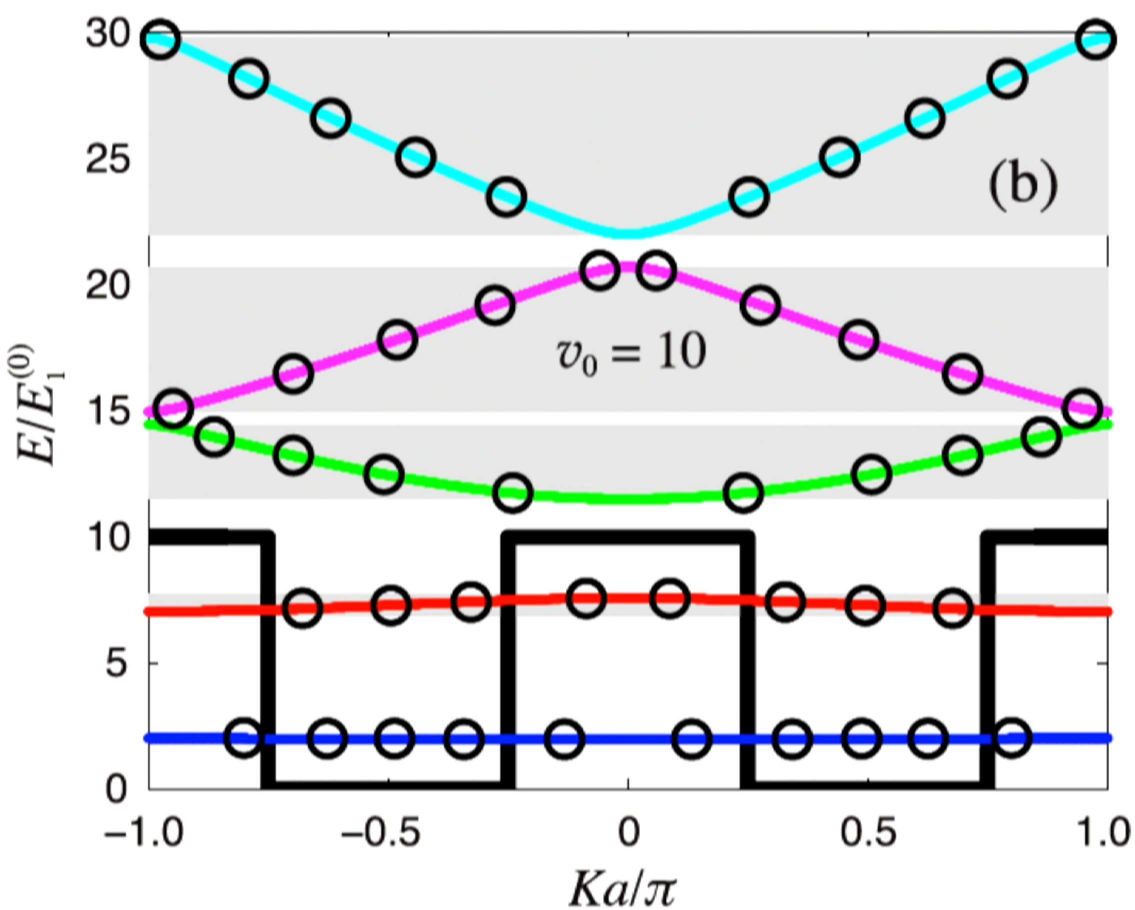

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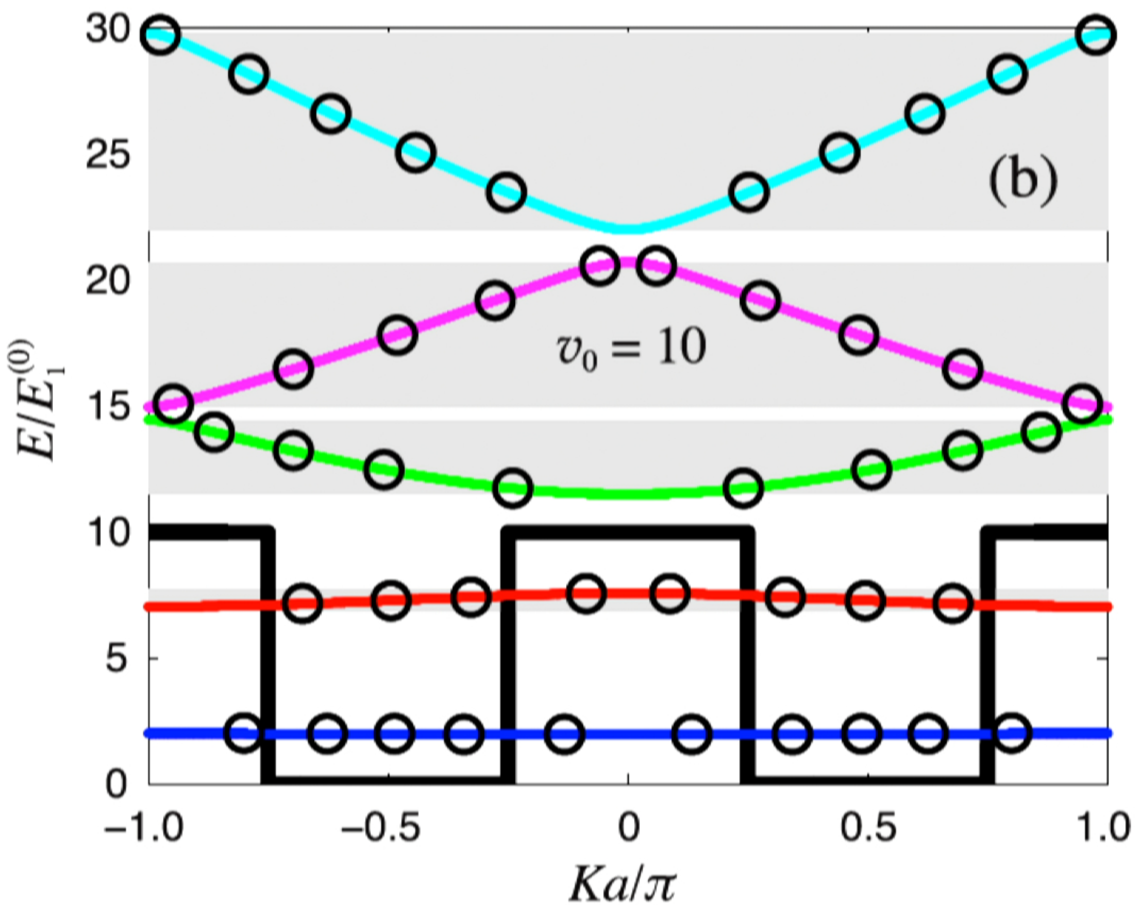

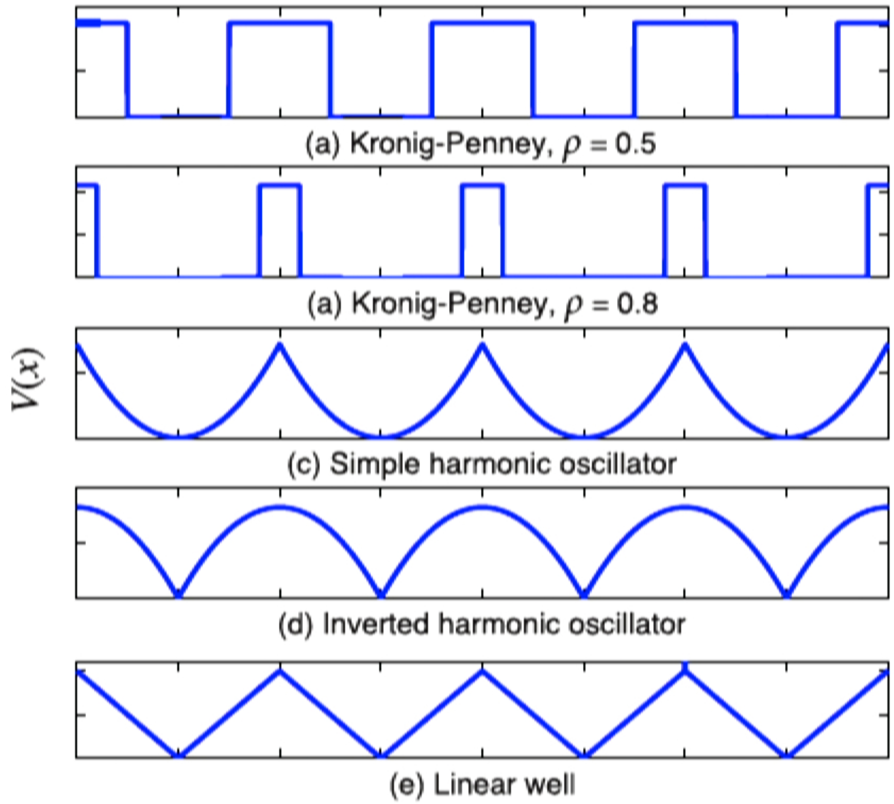

(a) Kronig-Penney, $\rho = 0.5$

(a) Kronig-Penney, $\rho = 0.8$

(c) Simple harmonic oscillator

(d) Inverted harmonic oscillator

(e) Linear well

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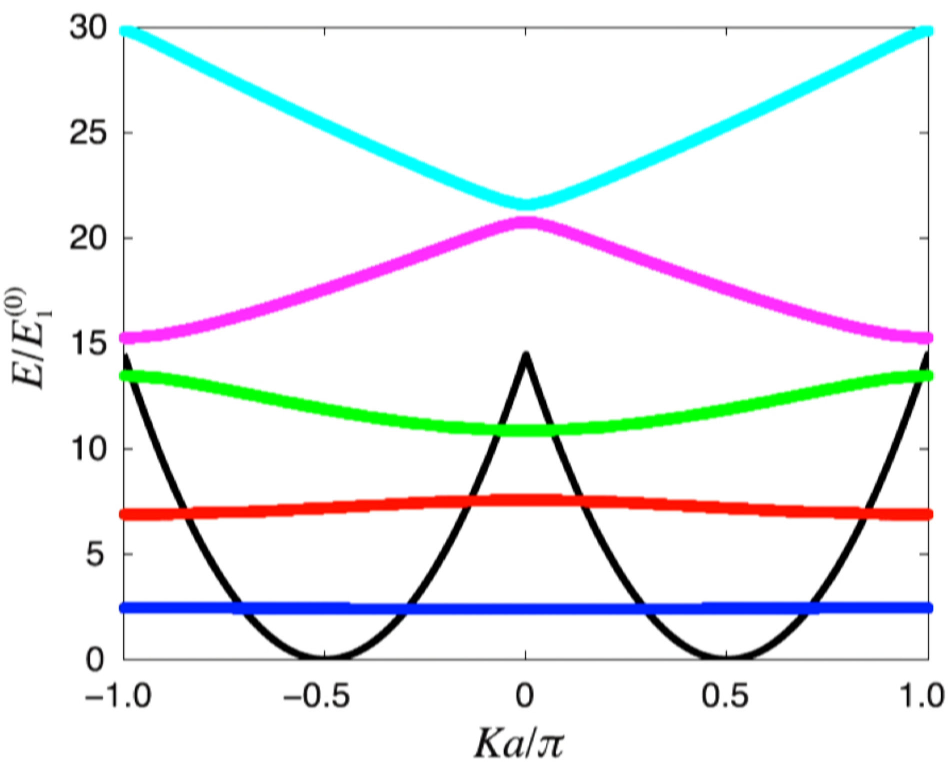

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Table I. The dimensionless second derivatives at the minimum (maximum) of the third energy bands from Fig. 11, which are inversely proportional to the electron and hole effective masses. The third column gives the ratio $e''_{\mathrm{e}}/e''_{\mathrm{h}} \equiv m^*_{\mathrm{h}}/m^*_{\mathrm{e}}$.

Potential	e''_{e}	e''_{h}	$m^*_{\mathrm{h}}/m^*_{\mathrm{e}}$
K-P ($\rho = 0.5$)	13.83	−25.35	−0.55
K-P ($\rho = 0.8$)	39.09	−70.61	−0.55
Simple HO	37.84	−121.80	−0.31
Inverted HO	19.83	−55.96	−0.35
Linear	31.63	−102.23	−0.31

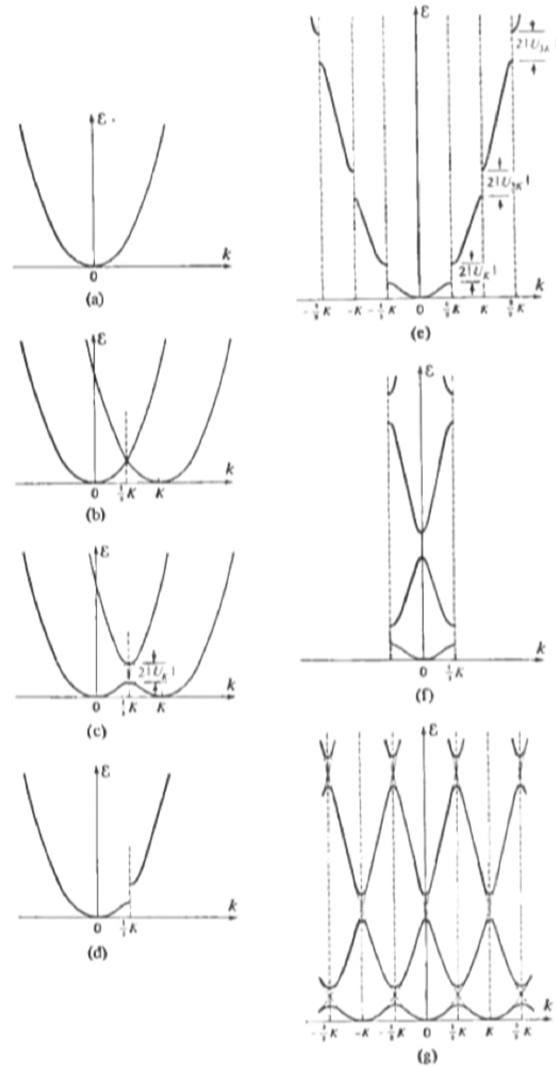

Figure 9.4
(a) The free electron ℰ vs. k parabola in one dimension. (b) Step 1 in the construction

Extended zone-scheme

in the neighborhood of a Bragg "plane," due to a weak periodic potential. If the Bragg "plane" is that determined by K, a second free electron parabola is drawn, centered on K. (c) Step 2 in the construction to determine the distortion in the free electron parabola in the neighborhood of a Bragg "plane." The degeneracy of the two parabolas at $K/2$

Reduced zone-scheme

parabola given in (a). (e) Effect of all additional Bragg "planes" on the free electron parabola. This particular way of displaying the electronic levels in a periodic potential is known as the *extended-zone scheme*. (f) The levels of (e), displayed in a *reduced-zone scheme*. (g) Free electron levels of (e) or (f) in a *repeated-zone scheme*.

Repeated zone-scheme

Fig. 9.4 from Ashcroft and Mermin

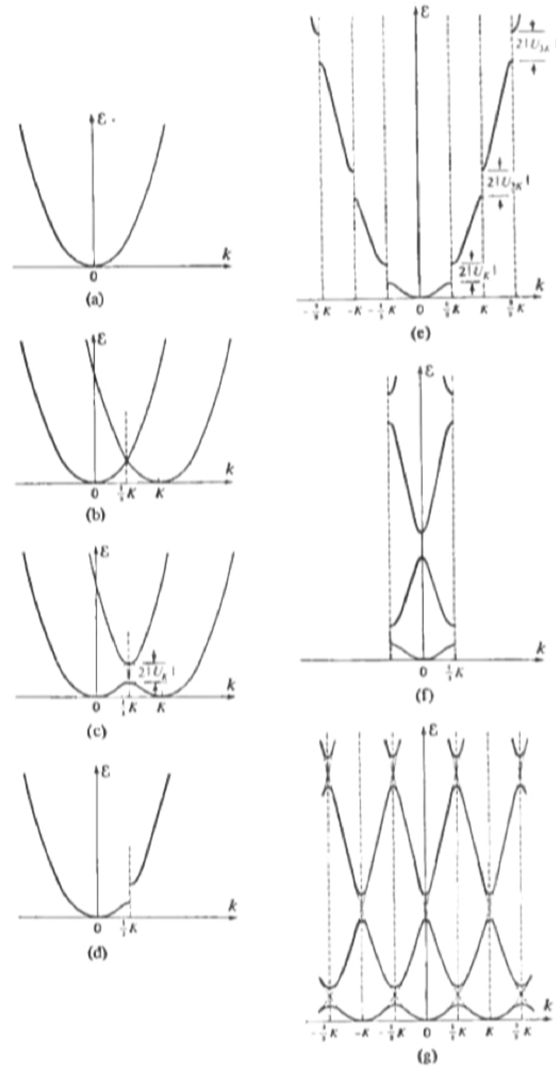

Figure 9.4
(a) The free electron $\mathcal{E}$ vs. k parabola in one dimension. (b) Step 1 in the construction

Extended zone-scheme

in the neighborhood of a Bragg "plane," due to a weak periodic potential. If the Bragg "plane" is that determined by K, a second free electron parabola is drawn, centered on K. (c) Step 2 in the construction to determine the distortion in the free electron parabola in the neighborhood of a Bragg "plane." The degeneracy of the two parabolas at $K/2$

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Repeated zone-scheme

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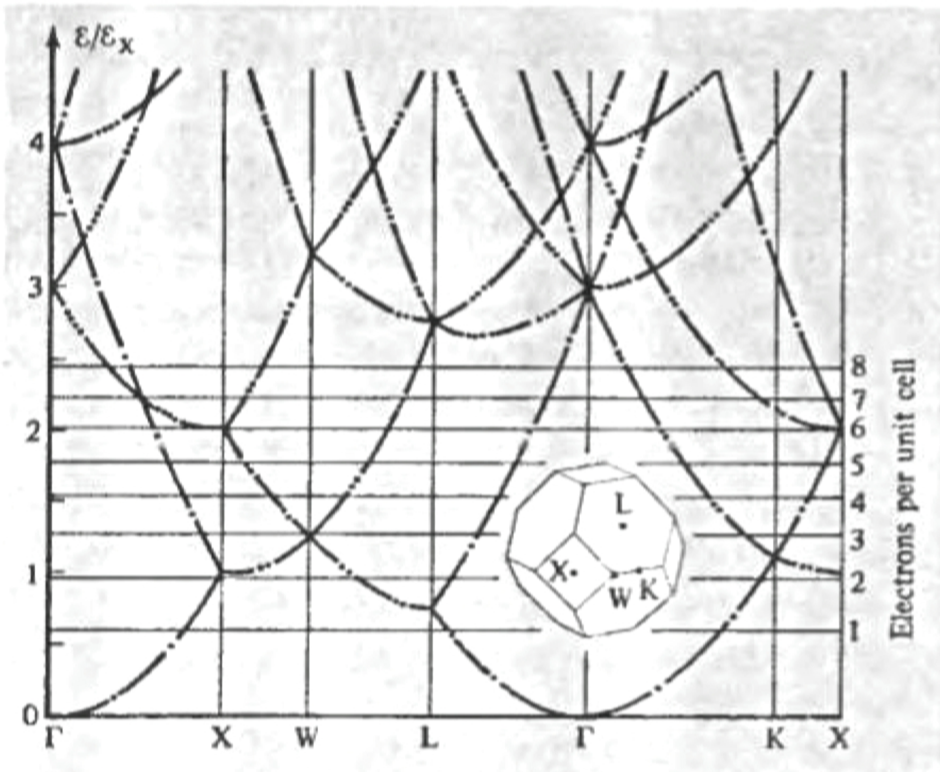

Figure 9.5
Free electron energy levels for an fcc Bravais lattice. The energies are plotted along lines in the first Brillouin zone joining the points $\Gamma(\mathbf{k} = 0)$, K, L, W, and X. $\mathcal{E}_x$ is the energy at point X $([\hbar^2/2m][2\pi/a]^2)$. The horizontal lines give Fermi energies for the indicated numbers of electrons per primitive cell. The number of dots on a curve specifies the number of degenerate free electron levels represented by the curve. (From F. Herman, in *An Atomistic Approach to the Nature and Properties of Materials*, J. A. Pask, ed., Wiley, New York, 1967.)

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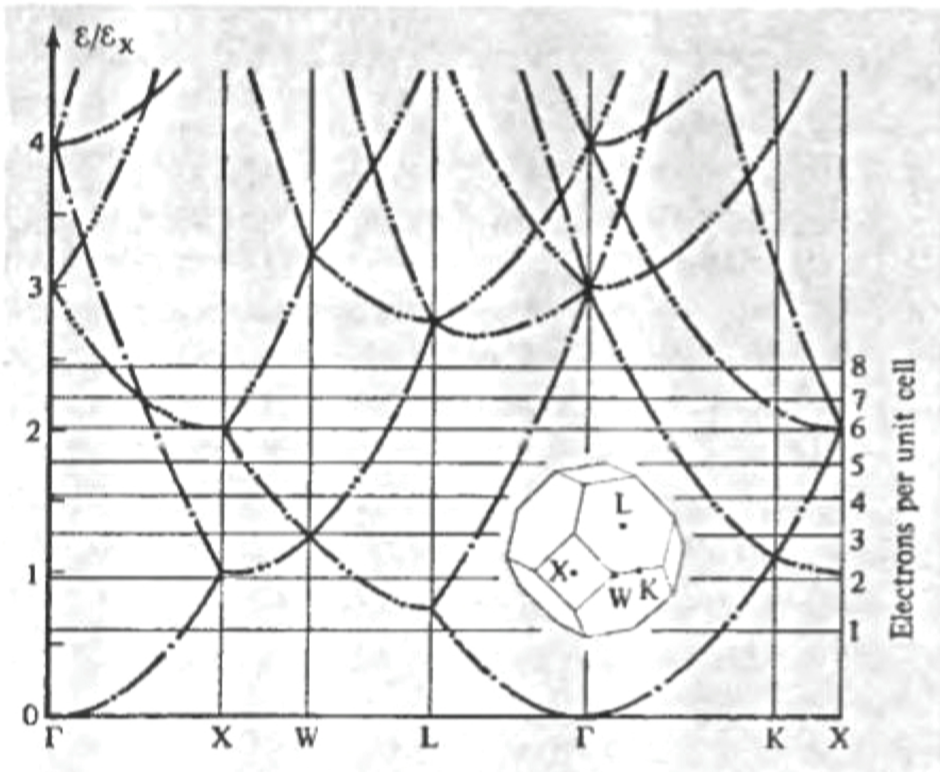

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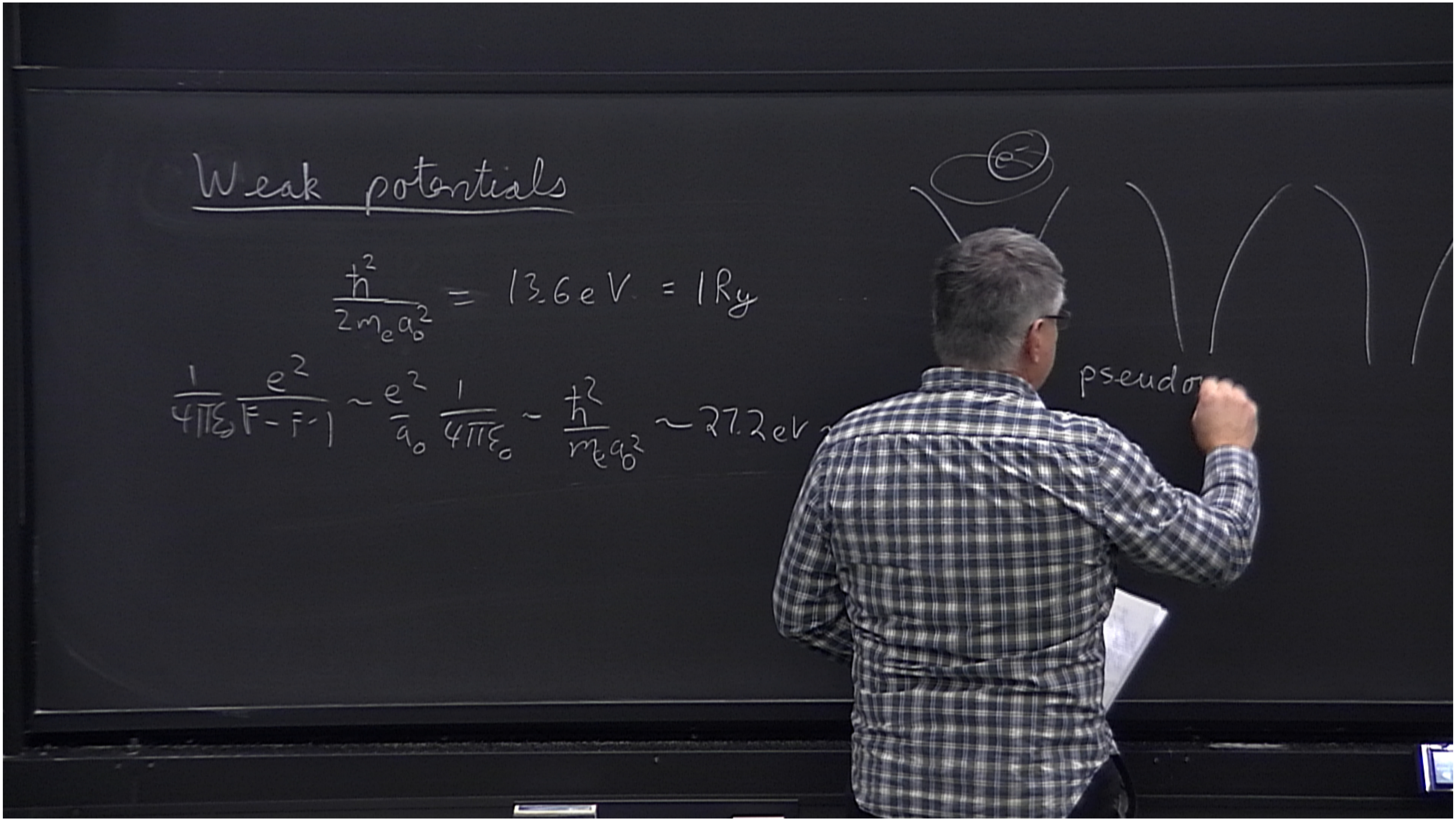
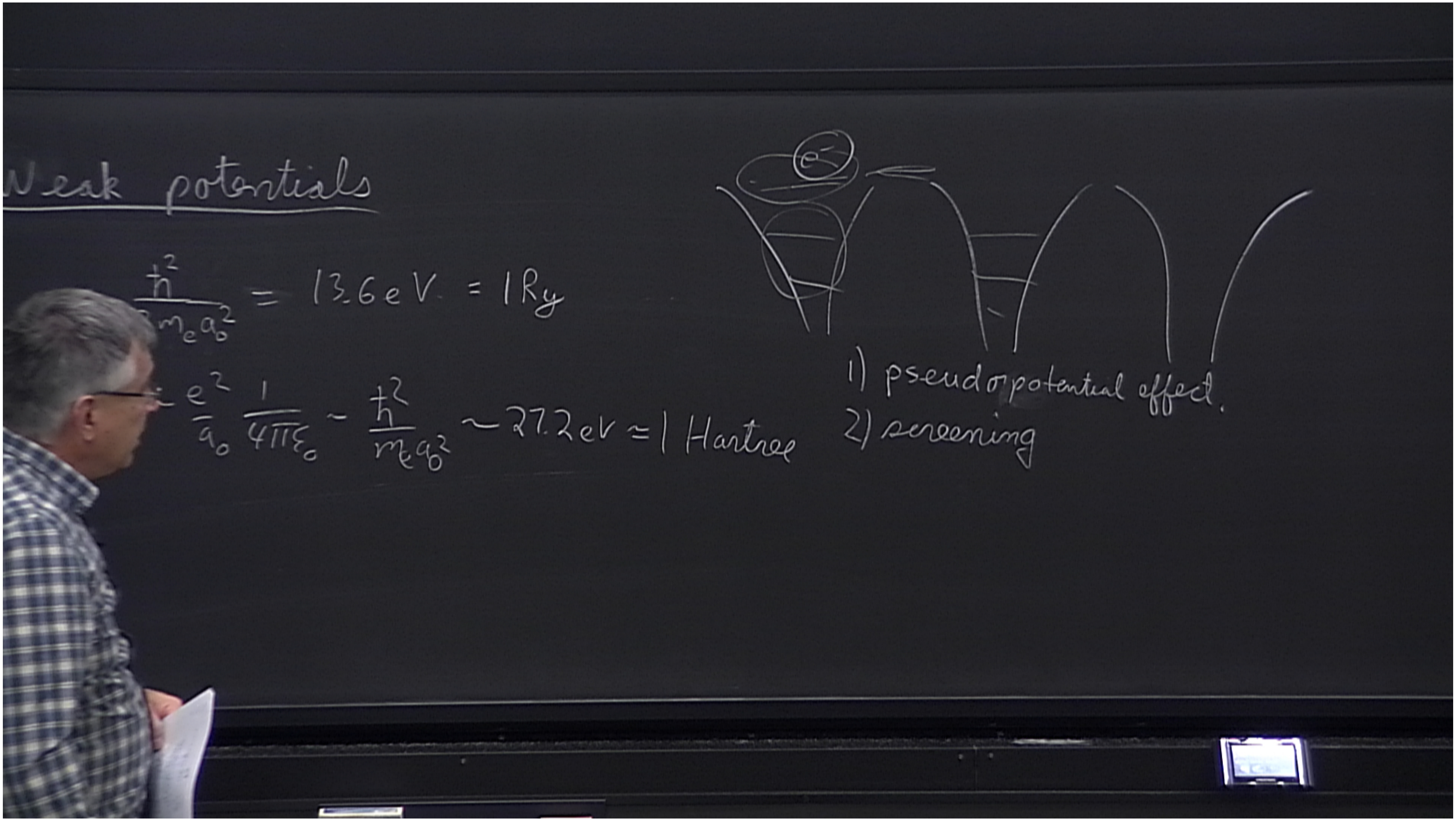
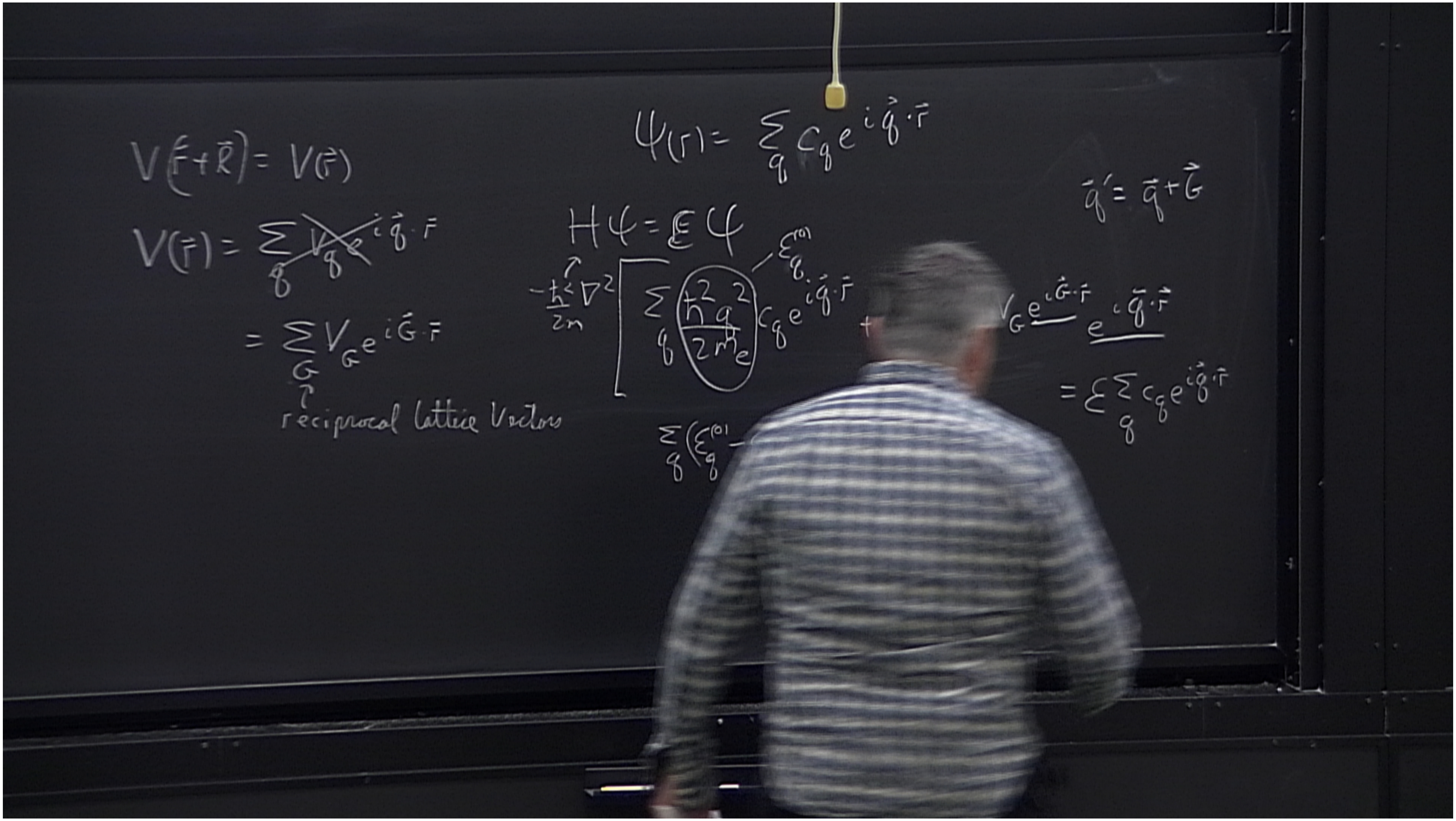

Weak potentials
$\frac{\hbar^2}{2m_e a_0^2} = 13.6\,eV = 1\,Ry$
$\frac{1}{4\pi\varepsilon_0}\frac{e^2}{|r-r'|} \sim \frac{e^2}{a_0}\frac{1}{4\pi\varepsilon_0} \sim \frac{\hbar^2}{m_e a_0^2} \sim 27.2\,eV$
e^-
pseudo


Weak potentials
$\frac{\hbar^2}{2m_e a_0^2} = 13.6\,eV = 1\,Ry$
$\frac{e^2}{a_0}\frac{1}{4\pi\epsilon_0} \sim \frac{\hbar^2}{m_e a_0^2} \sim 27.2\,eV \simeq 1$ Hartree
e^-
1) pseudopotential effect.
2) screening



$V(\vec{r}+\vec{R}) = V(\vec{r})$
$V(\vec{r}) = \sum_q \cancel{V_q e^{i\vec{q}\cdot\vec{r}}}$
$= \sum_G V_G e^{i\vec{G}\cdot\vec{r}}$
reciprocal lattice vectors
$\psi(r) = \sum_q c_q e^{i\vec{q}\cdot\vec{r}}$
$H\psi = \varepsilon\psi$
$-\frac{\hbar^2}{2m}\nabla^2$
$\sum_q \frac{\hbar^2 q^2}{2m_e} c_q e^{i\vec{q}\cdot\vec{r}}$
$\varepsilon_q^{(0)}$
$V_G e^{i\vec{G}\cdot\vec{r}} e^{i\vec{q}\cdot\vec{r}}$
$\vec{q}' = \vec{q} + \vec{G}$
$= \varepsilon \sum_q c_q e^{i\vec{q}\cdot\vec{r}}$
$\sum_q (\varepsilon_q^{(0)} -$

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

$$V(\vec{r}) = \sum_q \cancel{V_q e^{i}}\vec{q}\cdot\vec{r}$$

$$= \sum_{G} V_G e^{i\vec{G}\cdot\vec{r}}$$

reciprocal lattice vectors

$$\psi(r) = \sum_q c_q e^{i\vec{q}\cdot\vec{r}}$$

$$H\psi = \mathcal{E}\psi$$

$$-\frac{\hbar^2\nabla^2}{2m}\left[\sum_q \underbrace{\frac{\hbar^2 q^2}{2m_e}}_{\mathcal{E}^{(0)}_q} c_q e^{i\vec{q}\cdot\vec{r}} + \sum_q c_q \sum_G V_G \underline{e^{i\vec{G}\cdot\vec{r}}}\,\underline{e^{i\vec{q}\cdot\vec{r}}}\right.$$

$$= \mathcal{E}\sum_q c_q e^{i\vec{q}\cdot\vec{r}}$$

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

$$\sum_q (\mathcal{E}^{(0)}_q - \mathcal{E}) c_q e^{i\vec{q}\cdot\vec{r}} + \sum_{q'} c_{q'-G} \sum_G V_G \; e^{i\vec{q}'\cdot\vec{r}} = 0$$

$$\sum_q (\quad) e^{iq\cdot r} = 0$$

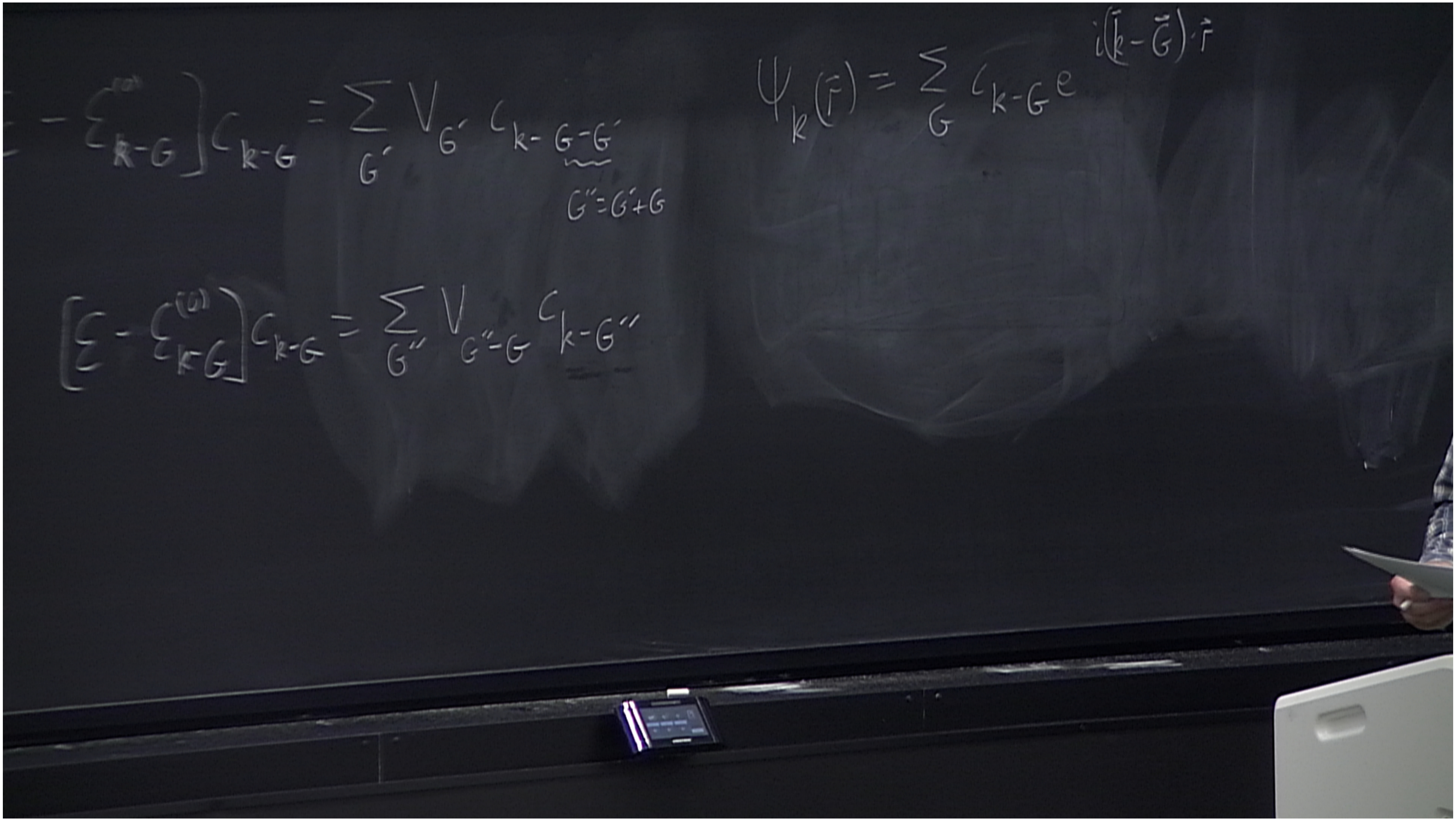
$$\left(\mathcal{E} - \mathcal{E}^{(0)}_q\right) c_q = \sum_{G'} V_{G'} c_{q-G'}$$

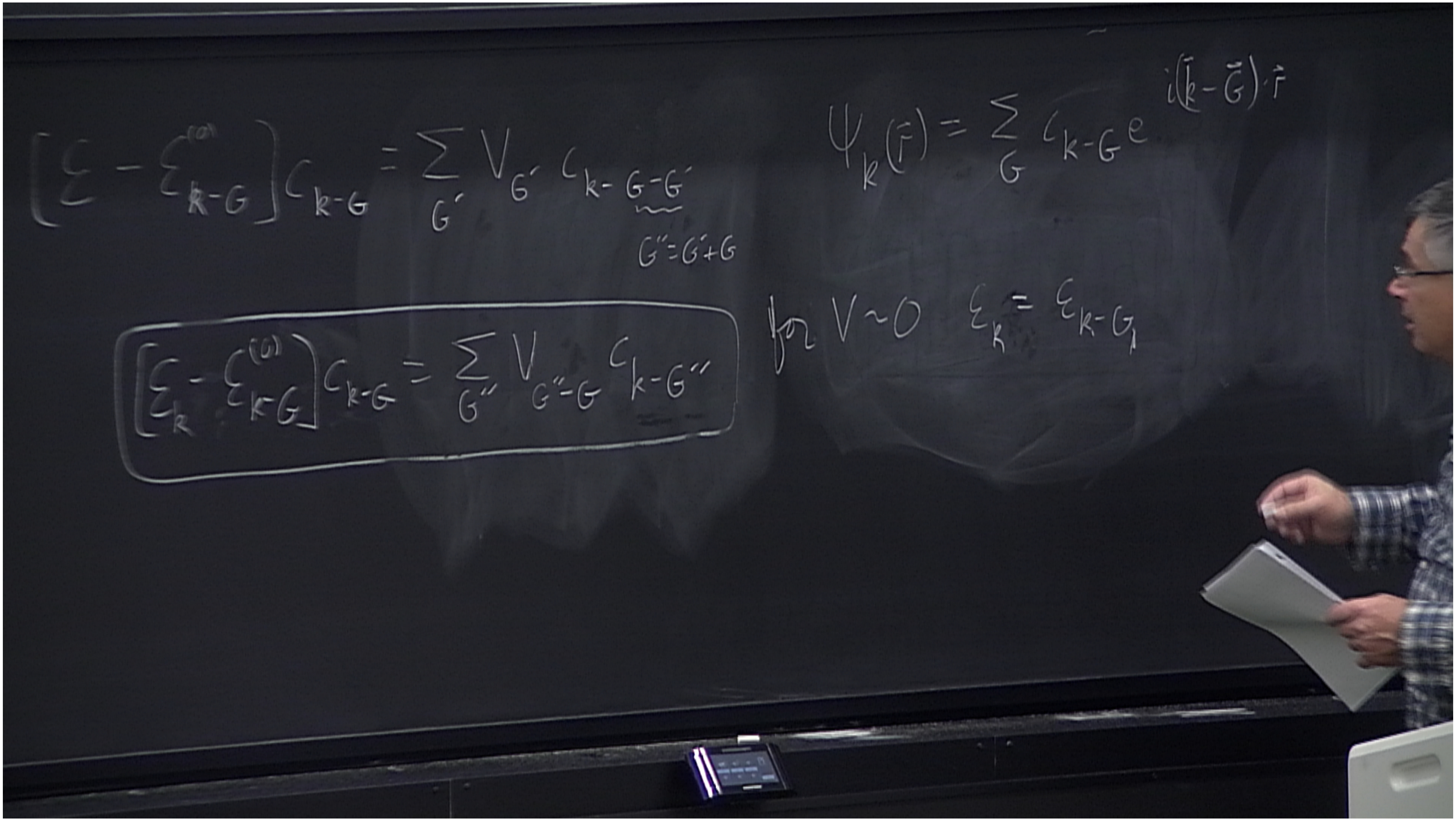
$q = k - G$

$\uparrow$

k is in FBZ

$$\left[\mathcal{E} - \mathcal{E}^{(0)}_{k-G}\right] c_{k-G} = \sum_{G'} V_{G'} c_{k-G}$$


$\left[\varepsilon - \varepsilon^{(0)}_{k-G}\right] c_{k-G} = \sum_{G'} V_{G'} c_{k-G-G'}$
$G'' = G' + G$
$\left[\varepsilon - \varepsilon^{(0)}_{k-G}\right] c_{k-G} = \sum_{G''} V_{G''-G} c_{k-G''}$
$\psi_k(\vec{r}) = \sum_G c_{k-G} e^{i(\vec{k}-\vec{G})\cdot\vec{r}}$



$\left[\varepsilon - \varepsilon^{(0)}_{k-G}\right] c_{k-G} = \sum_{G'} V_{G'} \, c_{k-G-G'}$
$G'' = G' + G$
$\psi_k(\vec{r}) = \sum_{G} c_{k-G} \, e^{i(\vec{k}-\vec{G})\cdot\vec{r}}$
$\boxed{\left[\varepsilon_k - \varepsilon^{(0)}_{k-G}\right] c_{k-G} = \sum_{G''} V_{G''-G} \, c_{k-G''}}$
for $V \sim 0$ $\varepsilon_k = \varepsilon_{k-G_1}$

$$\left[\varepsilon - \varepsilon^{(0)}_{k-G}\right] c_{k-G} = \sum_{G'} V_{G'}\, c_{k-\underbrace{G-G'}}$$

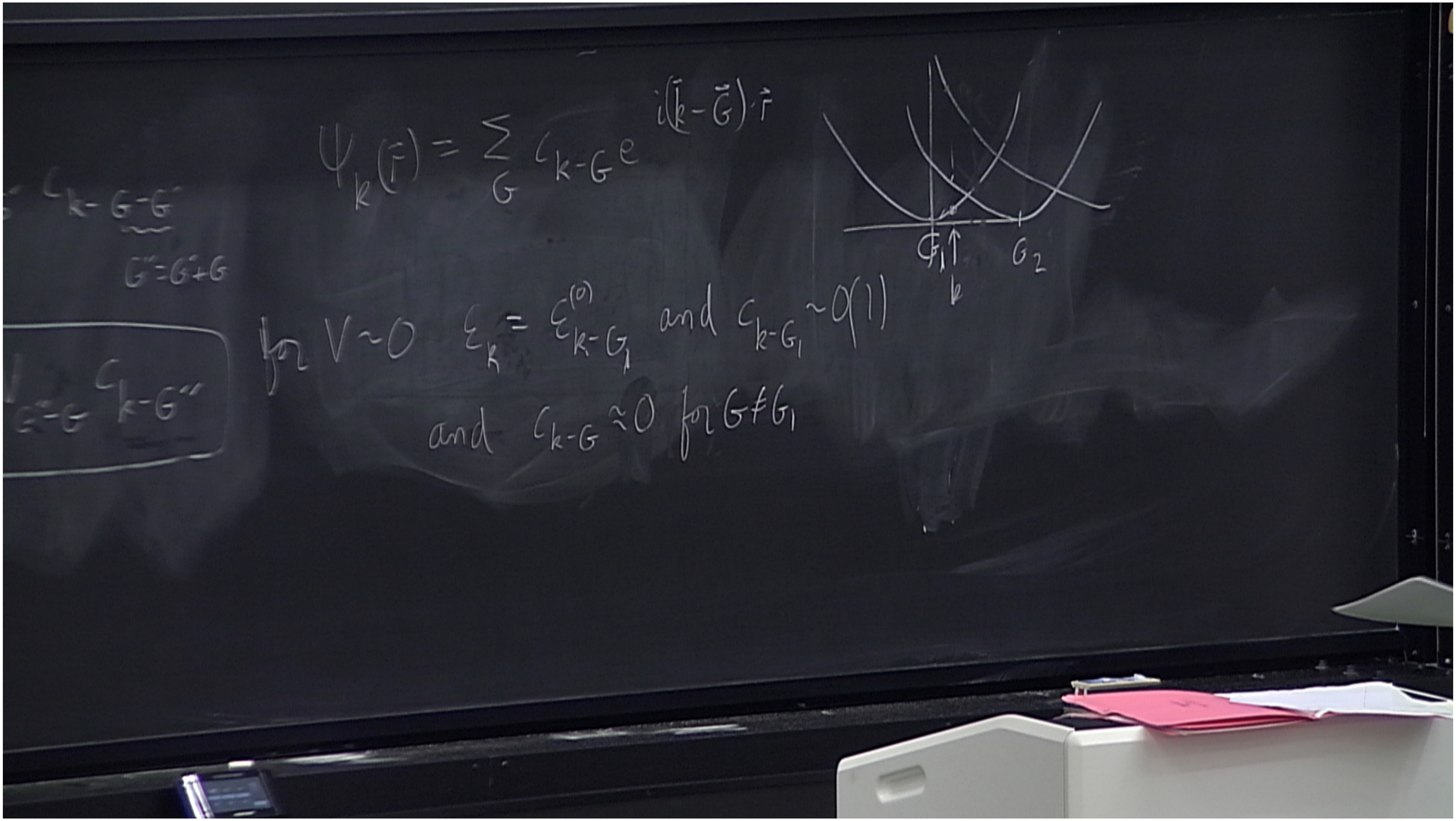
$$G'' = G' + G$$

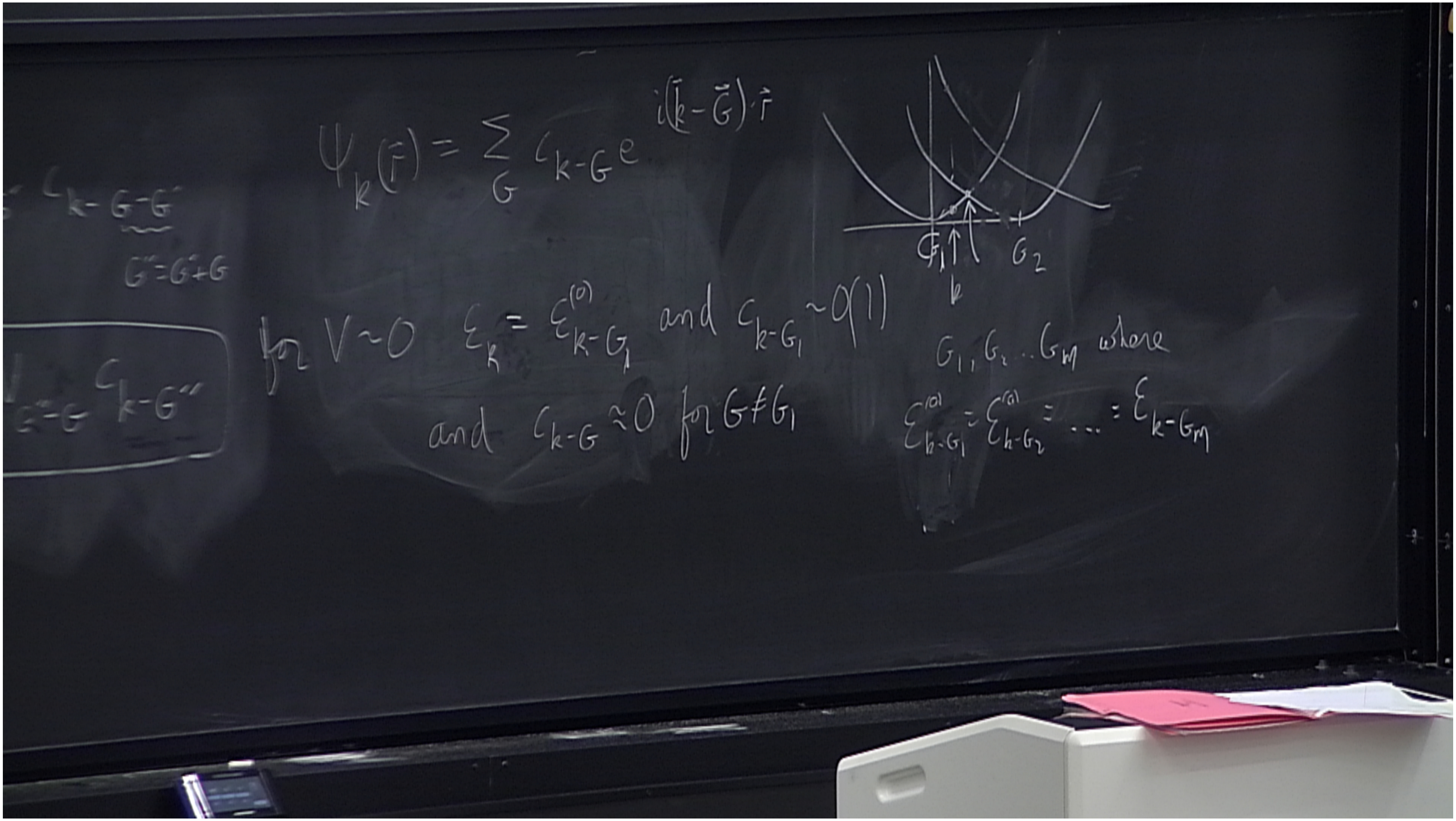
$$\boxed{\left[\varepsilon_k - \varepsilon^{(0)}_{k-G}\right] c_{k-G} = \sum_{G''} V_{G''-G}\, c_{k-G''}}$$

$$\psi_k(\vec{r}) = \sum_G c_{k-G}\, e^{i(\vec{k}-\vec{G})\cdot\vec{r}}$$

for $V \sim 0$ $\varepsilon_k = \varepsilon^{(0)}_{k-G_1}$ and $c_{k-G_1} \sim O(1)$

and $c_{k-G} \simeq 0$ for $G \neq G_1$


$\psi_k(\vec{r}) = \sum_G c_{k-G}\, e^{i(\vec{k}-\vec{G})\cdot\vec{r}}$
$c_{k-G-G'}$
$G''=G'+G$
$c_{k-G''}$
for $V\sim 0$ $\varepsilon_k = \varepsilon^{(0)}_{k-G_1}$ and $c_{k-G_1}\sim O(1)$
and $c_{k-G} \simeq 0$ for $G\neq G_1$
G_1
k
G_2


$c_{k-G-G'}$
$G''=G'+G$
$V_{G''-G}\, c_{k-G''}$
$\psi_k(\vec r) = \sum_G c_{k-G}\, e^{i(\vec k-\vec G)\cdot\vec r}$
G_1 k G_2
for $V\sim 0$ $\varepsilon_k = \varepsilon^{(0)}_{k-G_1}$ and $c_{k-G_1}\sim O(1)$
and $c_{k-G}\approx 0$ for $G\neq G_1$
$G_1, G_2 \ldots G_M$ where
$\varepsilon^{(0)}_{k-G_1} = \varepsilon^{(0)}_{k-G_2} = \ldots = \varepsilon_{k-G_M}$

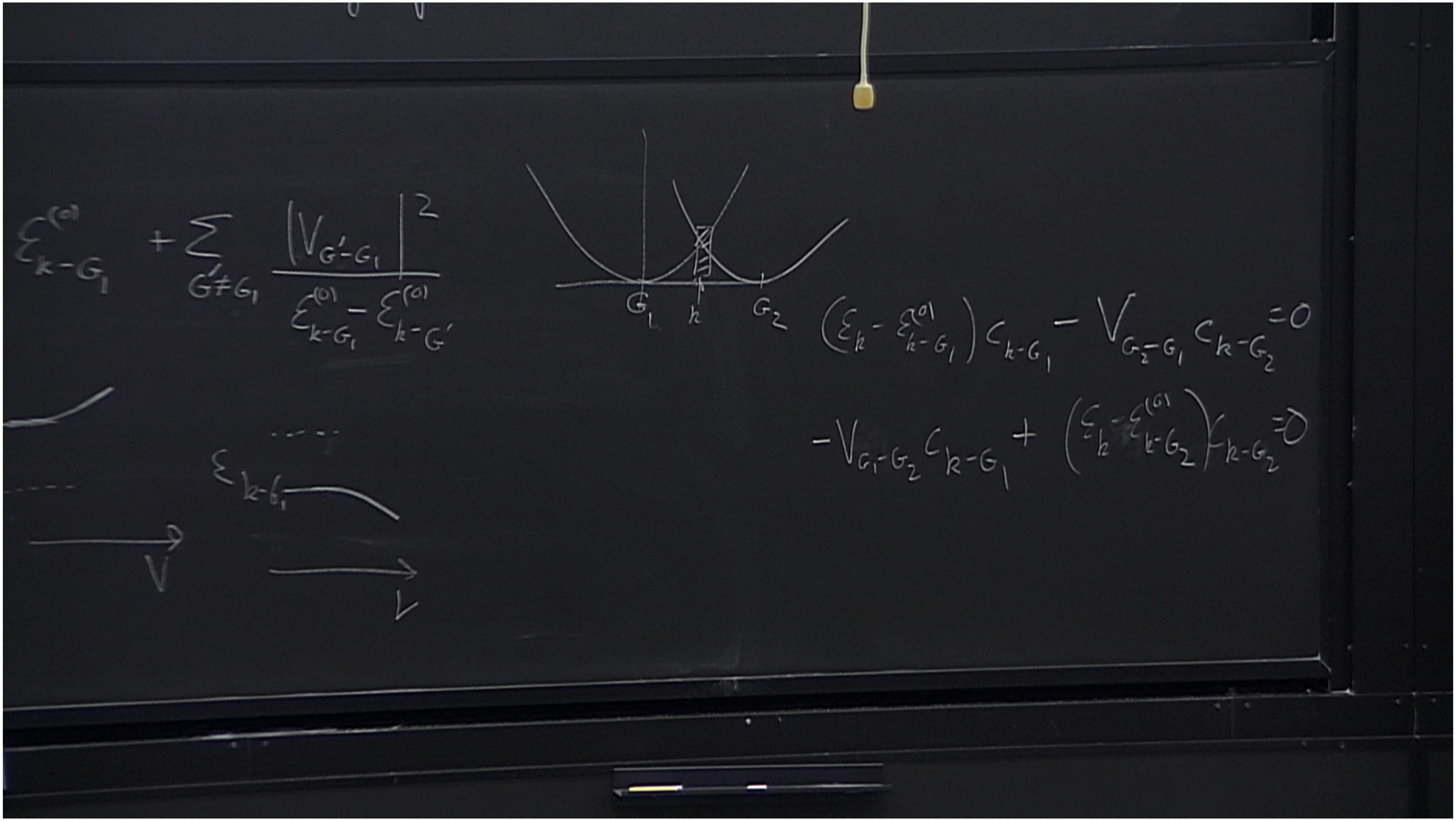
Case I

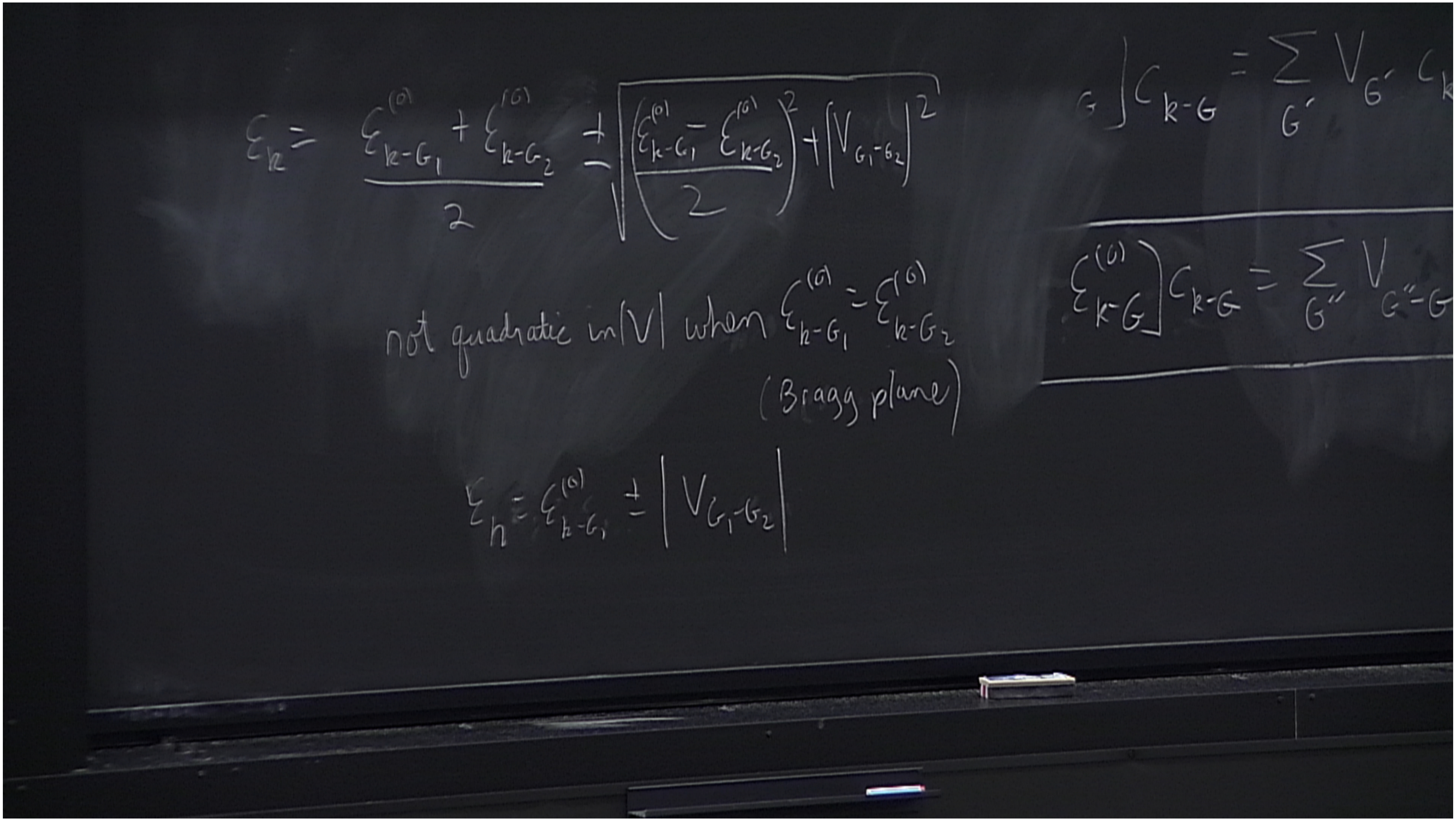
$\varepsilon_k \sim \varepsilon^{(0)}_{k-G_1}$

and all other $\varepsilon^{(0)}_{k-G}$ for $G \neq G_1$ are far away

$c_{k-G_1} \sim O(1)$

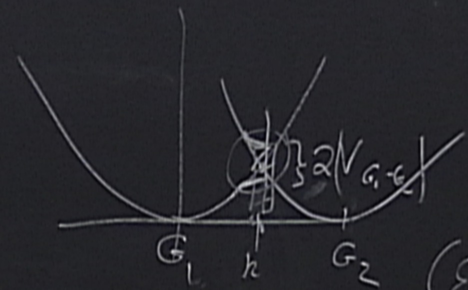
c_{k-G} for $G \neq G_1$ $\simeq$ small


$\mathcal{E}^{(0)}_{k-G_1} + \sum_{G' \neq G_1} \frac{|V_{G'-G_1}|^2}{\mathcal{E}^{(0)}_{k-G_1} - \mathcal{E}^{(0)}_{k-G'}}$
G_1
k
G_2
$(\mathcal{E}_k - \mathcal{E}^{(0)}_{k-G_1}) c_{k-G_1} - V_{G_2-G_1} c_{k-G_2} = 0$
$-V_{G_1-G_2} c_{k-G_1} + (\mathcal{E}_k - \mathcal{E}^{(0)}_{k-G_2}) c_{k-G_2} = 0$
$\mathcal{E}_{k-G_1}$
V
V



$\varepsilon_k = \frac{\varepsilon^{(0)}_{k-G_1}+\varepsilon^{(0)}_{k-G_2}}{2} \pm \sqrt{\left(\frac{\varepsilon^{(0)}_{k-G_1}-\varepsilon^{(0)}_{k-G_2}}{2}\right)^2 + \left|V_{G_1-G_2}\right|^2}$
not quadratic in $|V|$ when $\varepsilon^{(0)}_{k-G_1} = \varepsilon^{(0)}_{k-G_2}$
(Bragg plane)
$\varepsilon_k = \varepsilon^{(0)}_{k-G_1} \pm \left|V_{G_1-G_2}\right|$
$G \,]\, C_{k-G} = \sum_{G'} V_{G'} \, C_k$
$\left[\varepsilon^{(0)}_{k-G}\right] C_{k-G} = \sum_{G''} V_{G''-G}$

$$\varepsilon_k = \varepsilon^{(0)}_{k-G_1} + \sum_{G' \neq G_1} \frac{\left|V_{G'-G_1}\right|^2}{\varepsilon^{(0)}_{k-G_1} - \varepsilon^{(0)}_{k-G'}}$$



$$\left(\varepsilon_k - \varepsilon^{(0)}_{k-G_1}\right) c_{k-G_1} - V_{G_2-G_1} c_{k-G_2} = 0$$

$$-V_{G_1-G_2} c_{k-G_1} + \left(\varepsilon_k - \varepsilon^{(0)}_{k-G_2}\right) c_{k-G_2} = 0$$