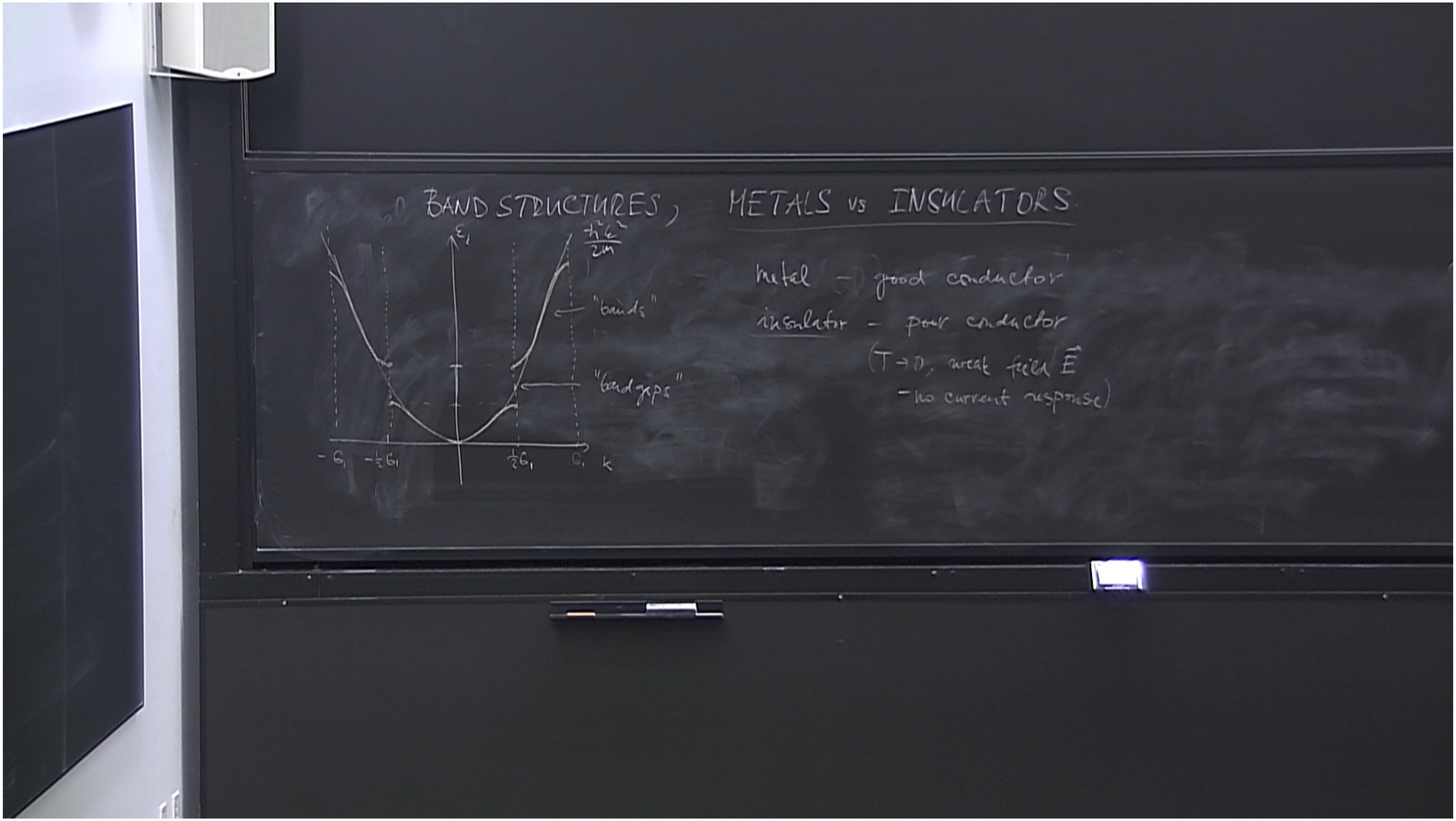
Title: 14/15 PSI - Condensed Matter-Lecture 9

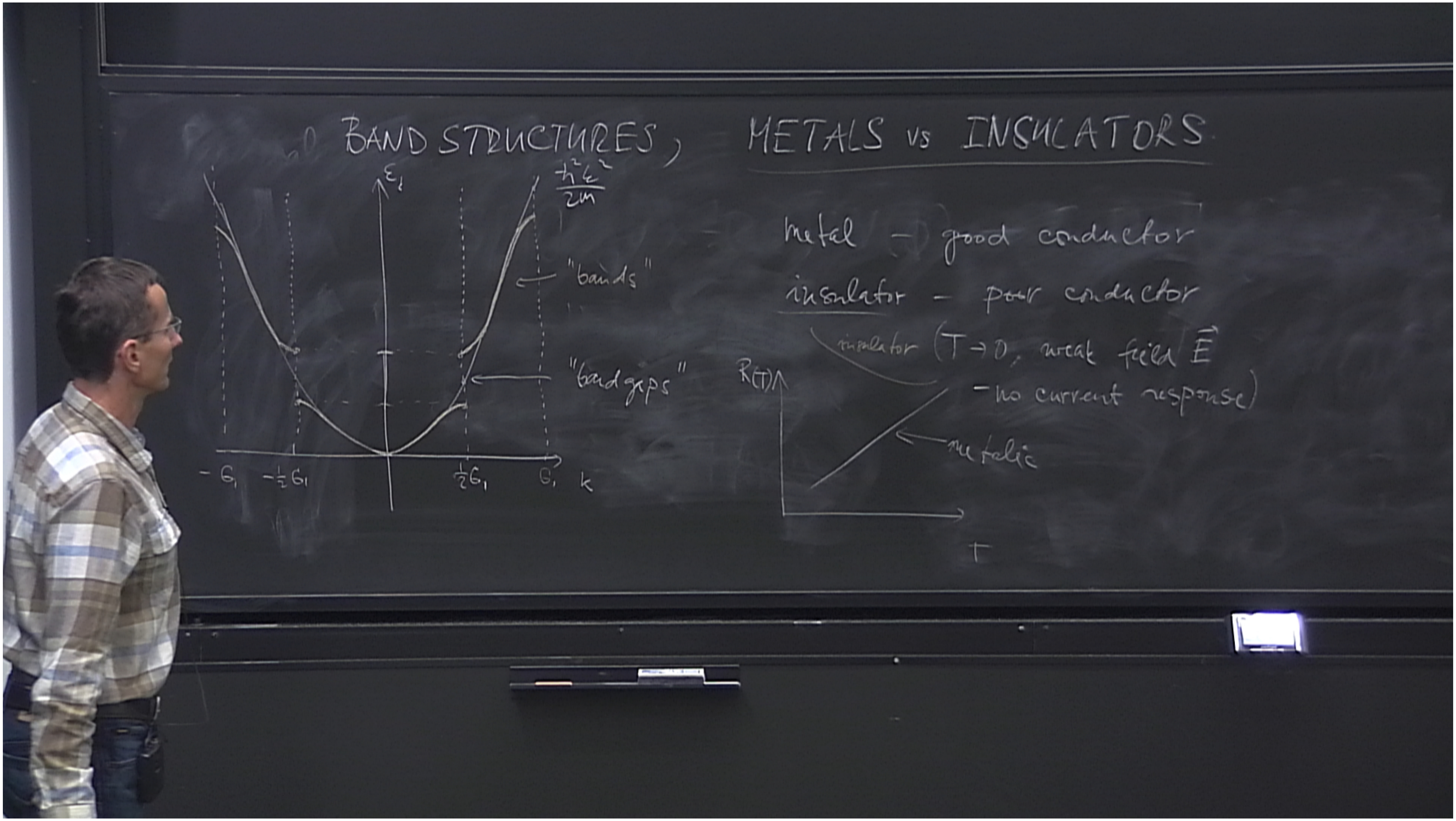
Date: Nov 20, 2014 10:45 AM

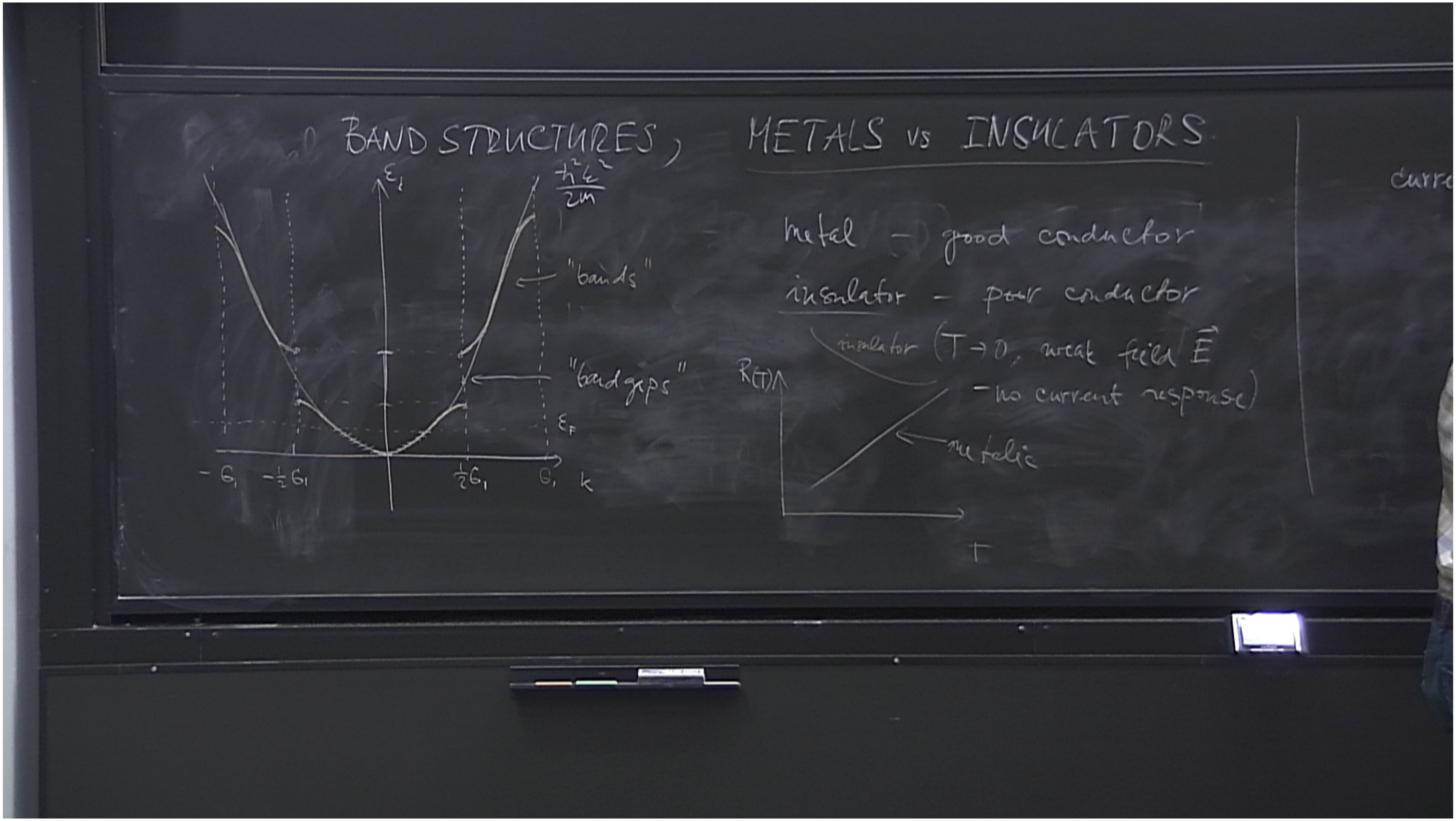
URL: http://pirsa.org/14110035

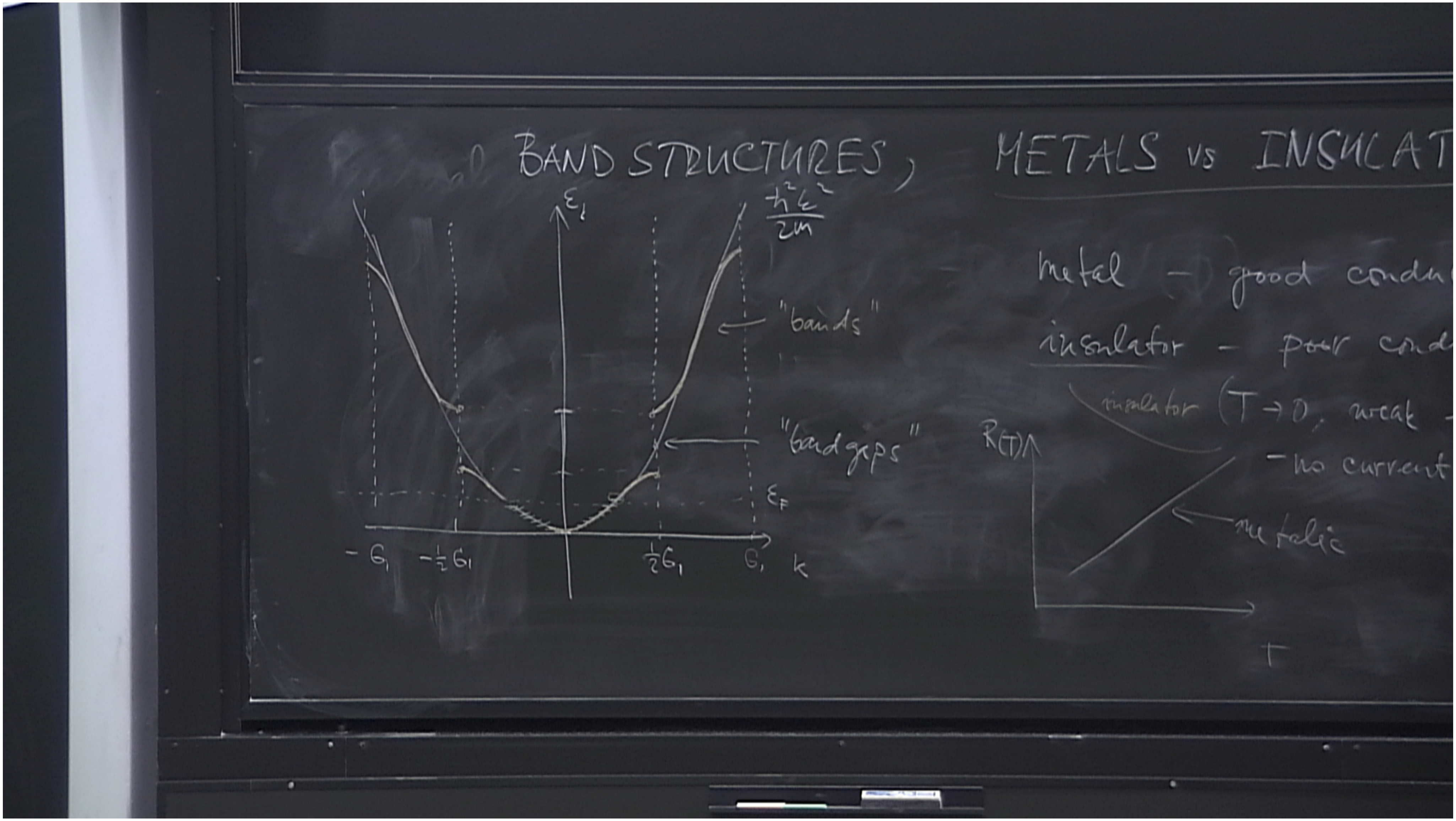
Abstract:


BAND STRUCTURES, METALS vs INSULATORS
ε_1
$-G_1$ $-\frac{1}{2}G_1$ $\frac{1}{2}G_1$ G_1 k


BAND STRUCTURES, METALS vs INSULATORS
"bands"
"band gaps"
metal - good conductor
insulator - poor conductor
(T→0, weak field E
- no current response)


BAND STRUCTURES,
METALS vs INSULATORS
ε_k
$\frac{\hbar^2 k^2}{2m}$
"bands"
"band gaps"
$-G_1$ $-\frac{1}{2}G_1$ $\frac{1}{2}G_1$ G_1 k
metal – good conductor
insulator – poor conductor
insulator (T → 0, weak field $\vec{E}$
– no current response)
R(T)
metallic
T


BAND STRUCTURES, METALS vs INSULATORS
ε_k
ħ²k²/2m
"bands"
"band gaps"
ε_F
−G₁ −½G₁ ½G₁ G₁ k
metal – good conductor
insulator – poor conductor
insulator (T → 0, weak field E
– no current response)
R(T)
metalic
T
curre



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metal — good condu
insulator — poor cond
insulator (T → 0, weak
R(T)
— no current
metalic
T

current: $\vec{j} = -e \sum_{k \in occ} \vec{v}(\vec{k})$, $\vec{v}(\vec{k}) = \frac{1}{\hbar} \frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}}$

- Metals are solids with partially filled bands (easy to produce current)

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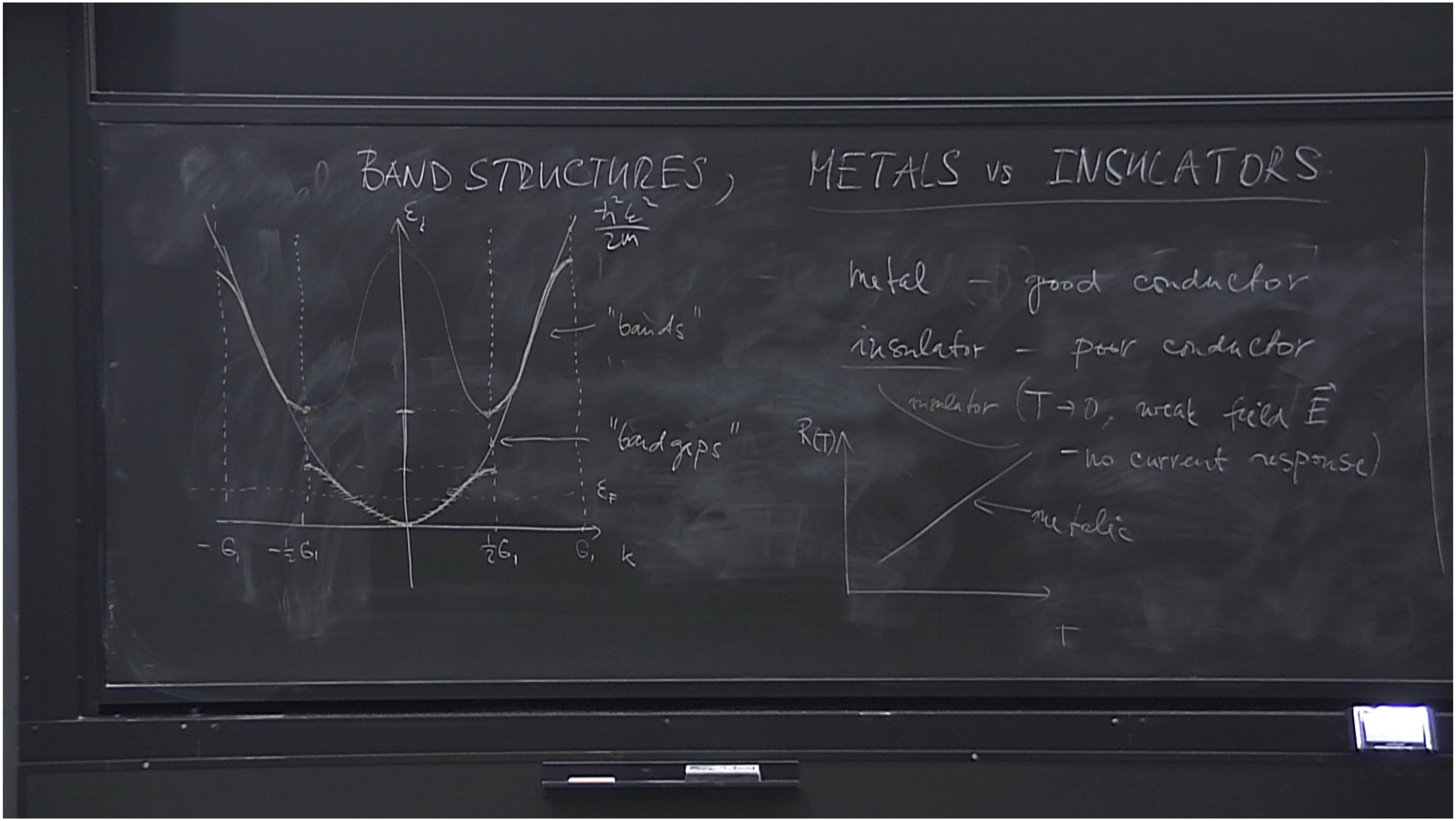
- Metals are solids with partially filled bands (easy to produce current)

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

$$v(k) = \frac{\hbar k}{m}$$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ε_k
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"bands"
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metal – good conductor
insulator – poor conductor
insulator ($T \to 0$, weak field $\vec{E}$
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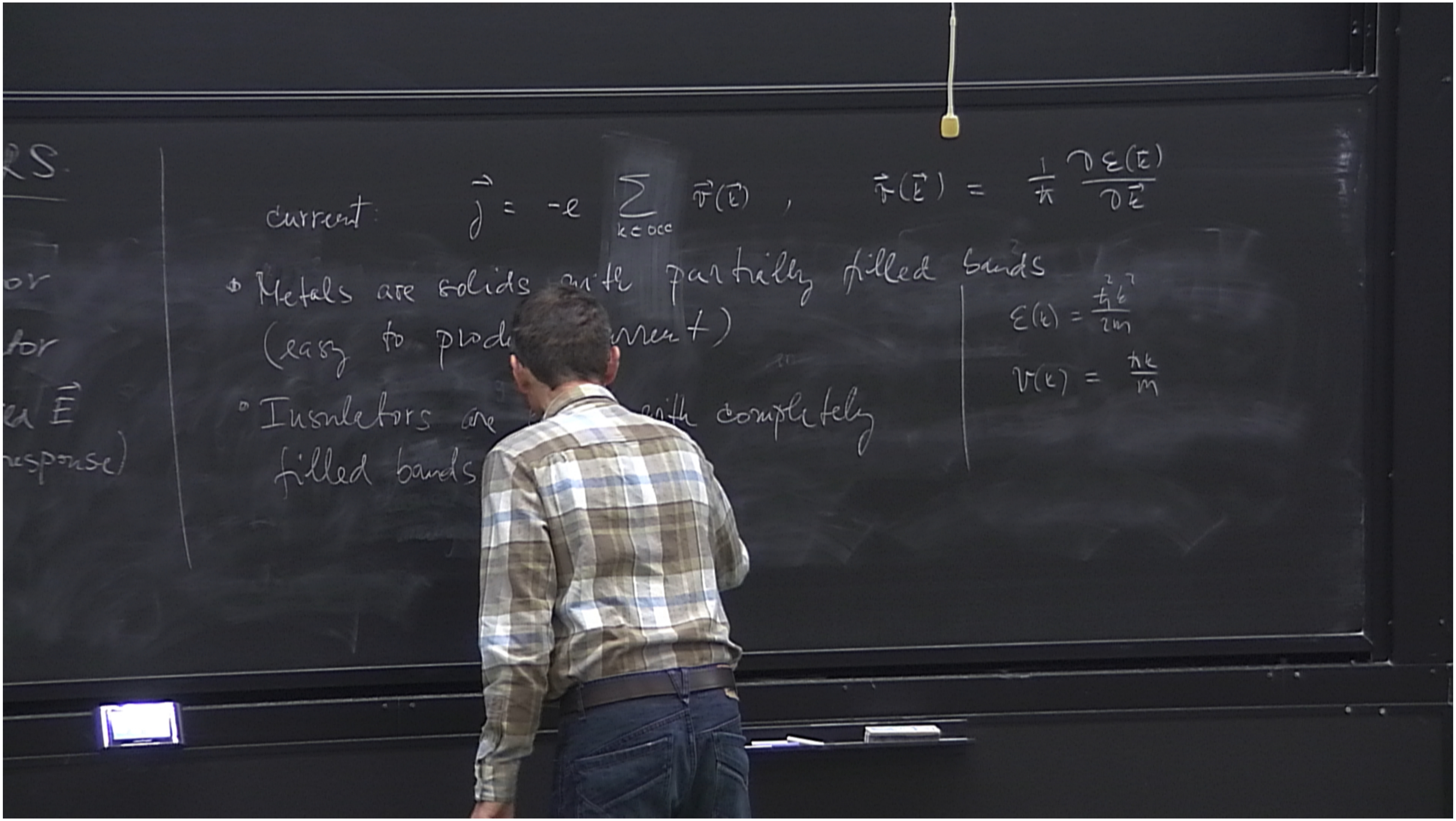
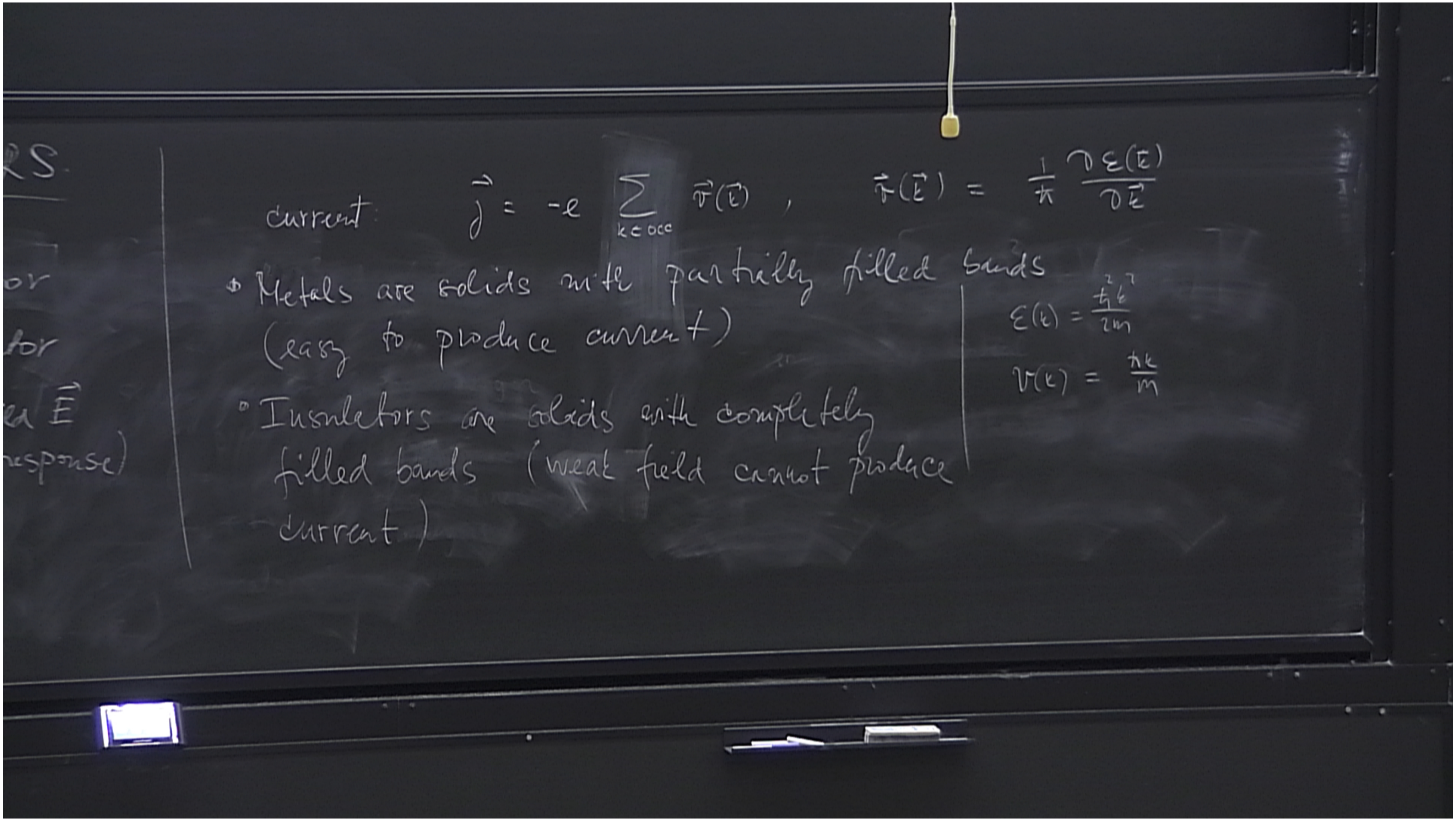
$R(T)$
metalic
T


current: $\vec{j} = -e \sum_{k \in occ} \vec{v}(\vec{k})$, $\vec{v}(\vec{k}) = \frac{1}{\hbar}\frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}}$
Metals are solids with the partially filled bands
(easy to
current)
Insulators are
with completely
filled bands
$\varepsilon(k) = \frac{\hbar^2 k^2}{2m}$
$v(k) = \frac{\hbar k}{m}$


current: $\vec{j} = -e \sum_{k \in occ} \vec{v}(\vec{k})$, $\vec{v}(\vec{k}) = \frac{1}{\hbar} \frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}}$
• Metals are solids with partially filled bands (easy to produce current)
• Insulators are solids with completely filled bands (weak field cannot produce current)
$\varepsilon(k) = \frac{\hbar^2 k^2}{2m}$
$v(k) = \frac{\hbar k}{m}$

# of allowed $\vec{k}$-values in the BZ
is equal to the # N of unit
cells in the crystal.

$\Rightarrow$ One needs an even # of electrons
per unit cell to have an insulator.

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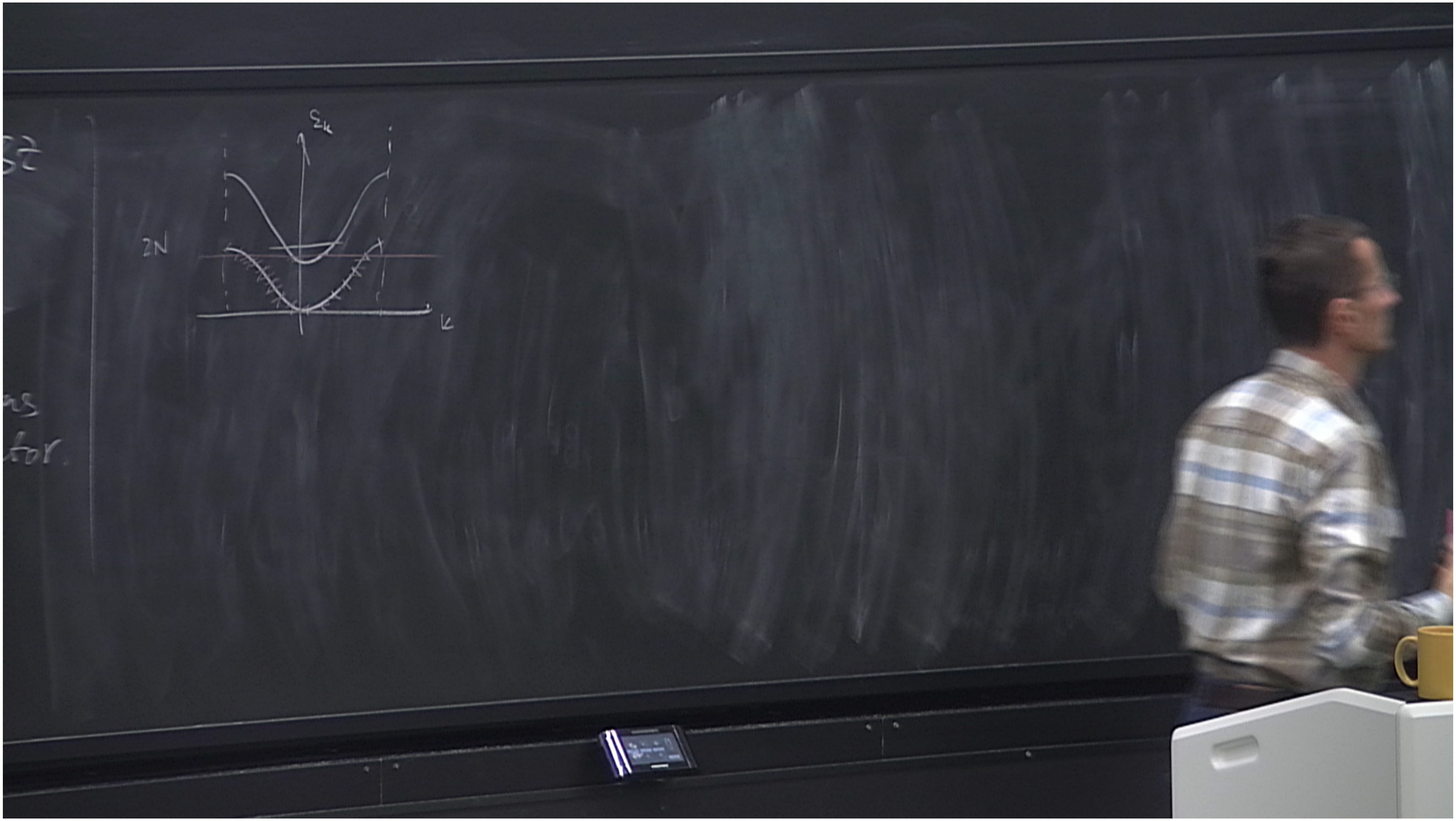
(necessary but not sufficient
condition)


ε_k
2N
k

Some magnon data

MAGNONS, CH. 4 53

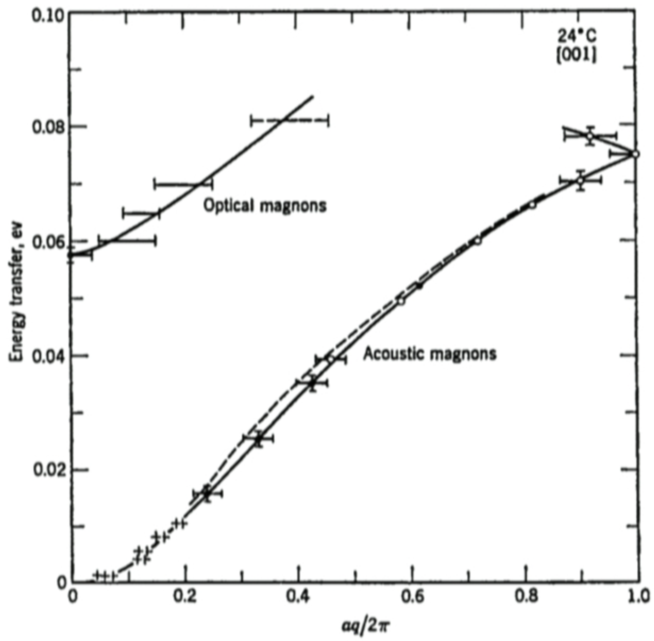


FIG. 1. Acoustical and optical magnon dispersion relations in magnetite, as determined from inelastic neutron scattering by Brockhouse and Watanabe (IAEA Symposium, Chalk River, Ontario, 1962).

56 QUANTUM THEORY OF SOLIDS

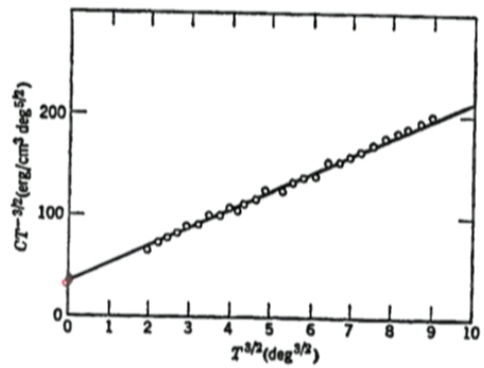
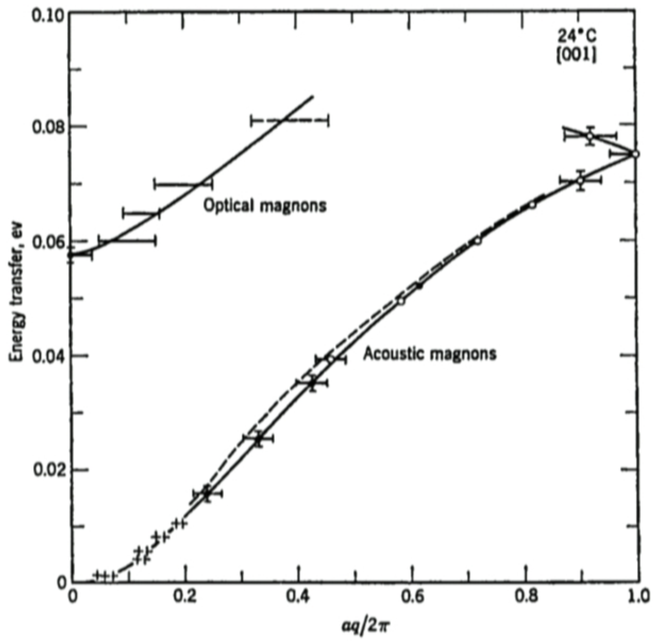


FIG. 2. Heat capacity of yttrium iron garnet, showing magnon and phonon contributions. (After Shinozaki.) The intercept at $T = 0$ measures the magnon contribution.

Some magnon data

MAGNONS, CH. 4 53



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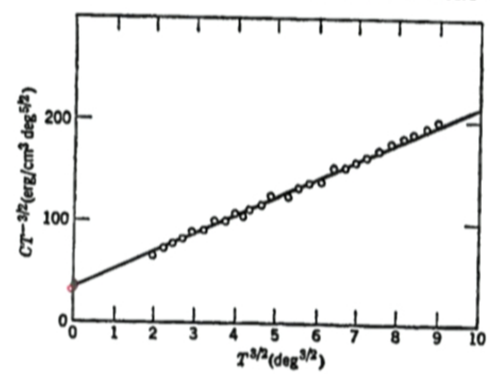

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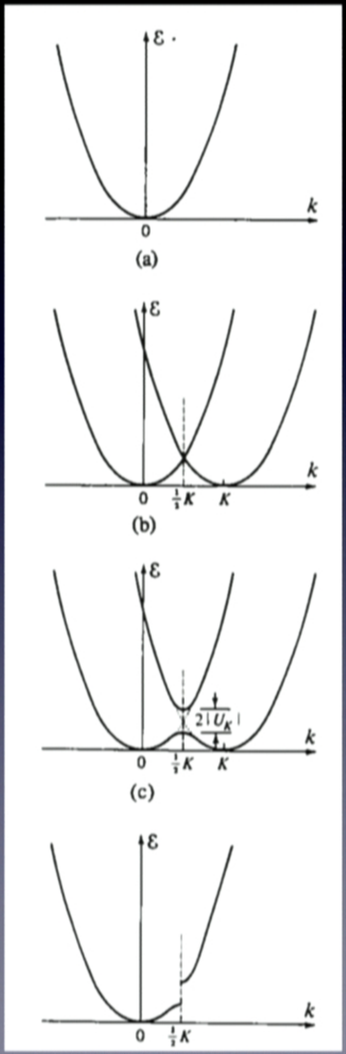
Weak periodic potential construction in 1D



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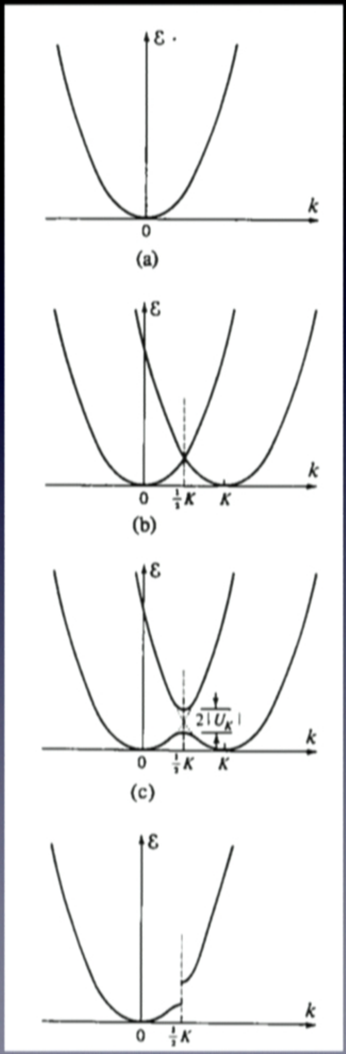

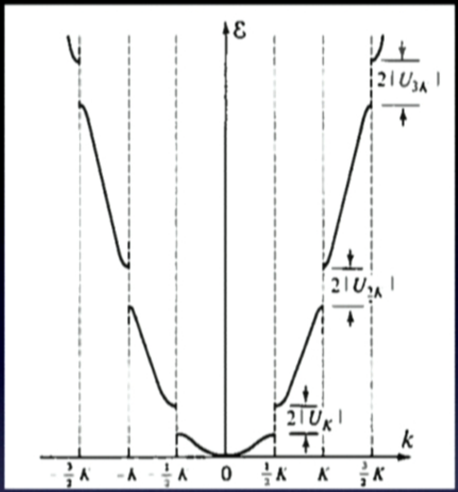

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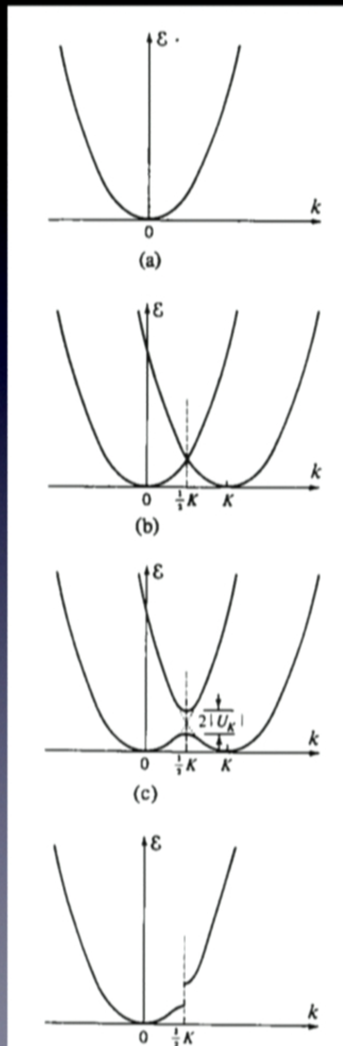
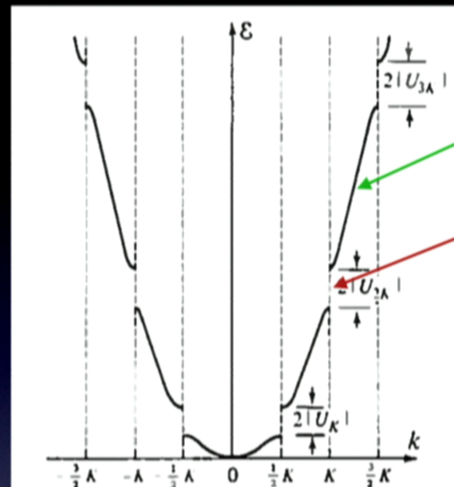
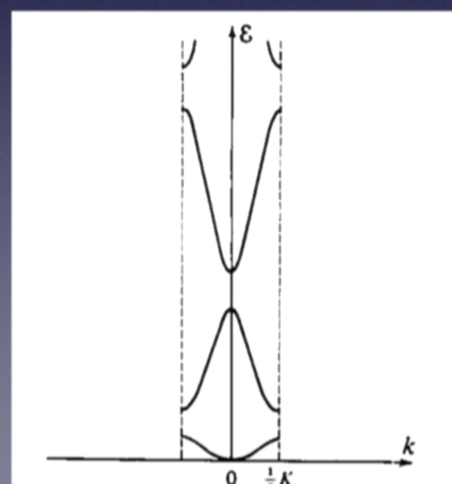




band

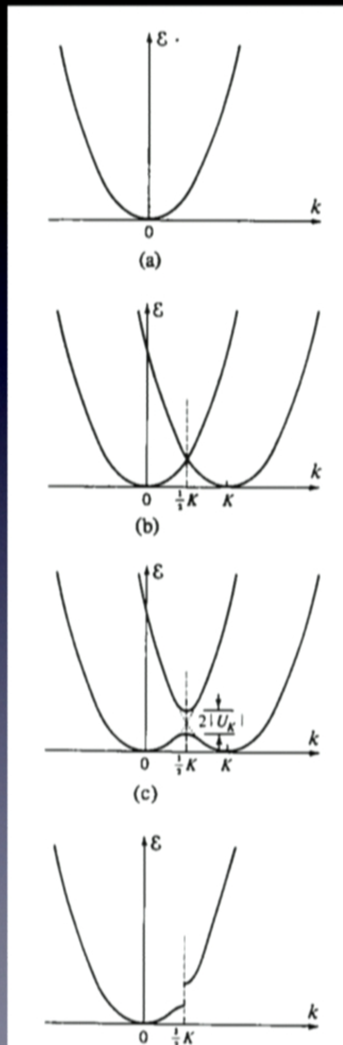
bandgap

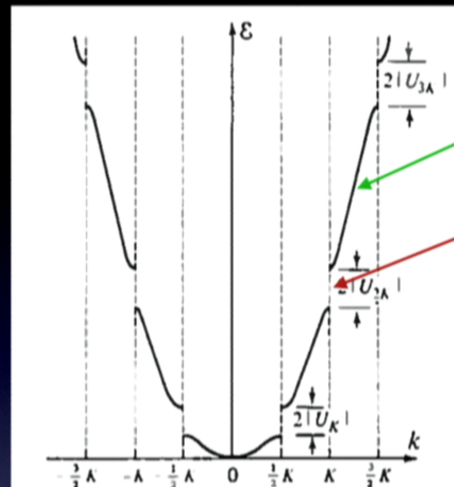
“extended zone scheme”



“reduced zone scheme”
(bands folded to the 1st Brillouin zone)

Weak periodic potential construction in 1D





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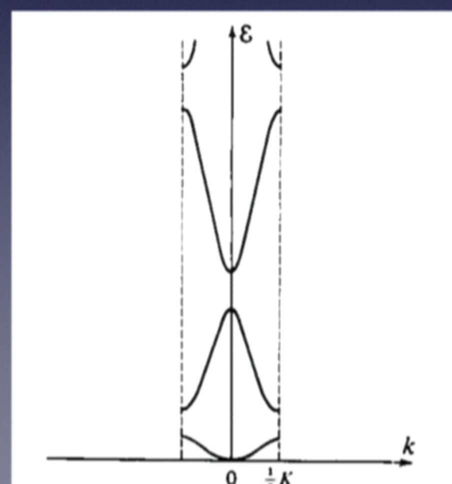

“reduced zone scheme”
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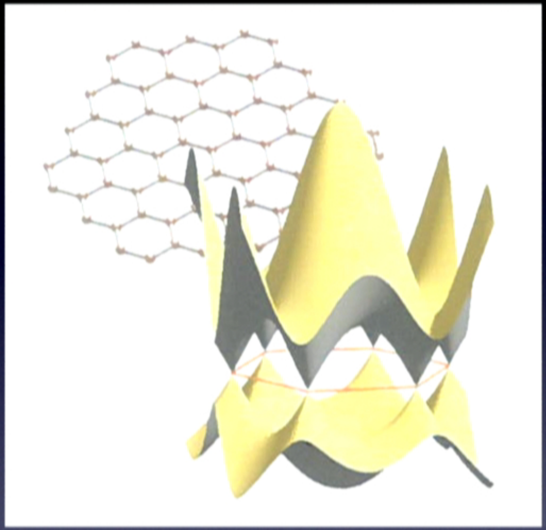
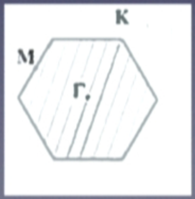
Graphene: example of a 2D band structure



1st Brillouin zone



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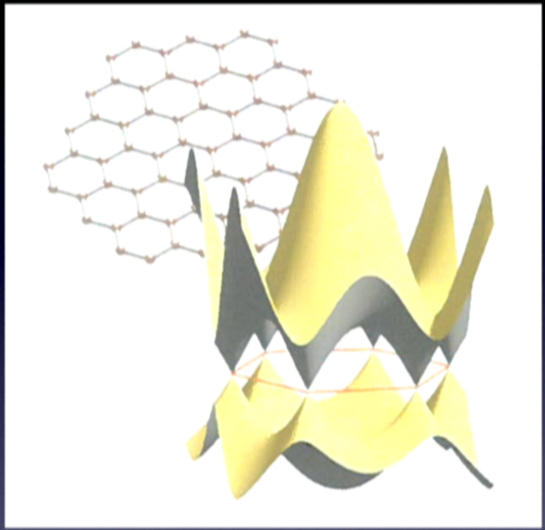

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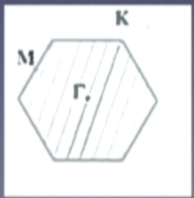

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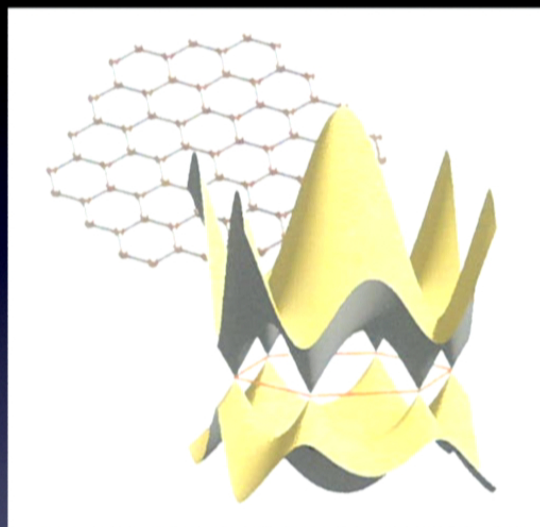

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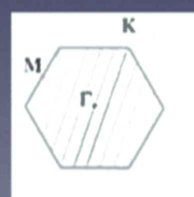

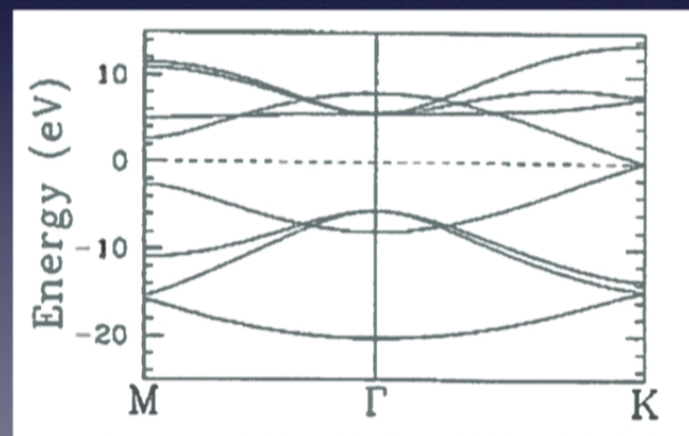

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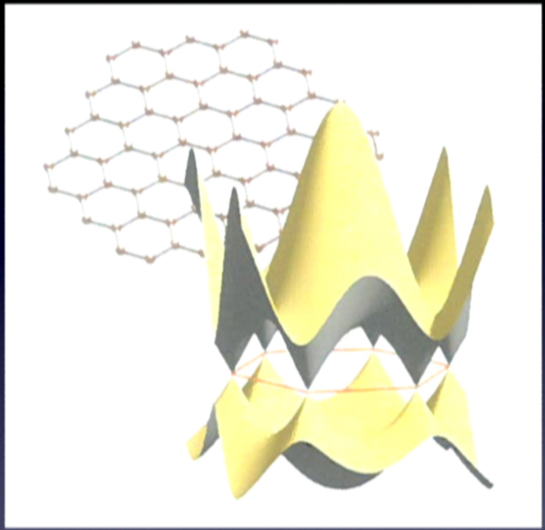

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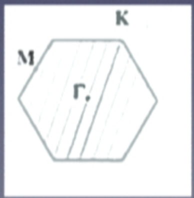

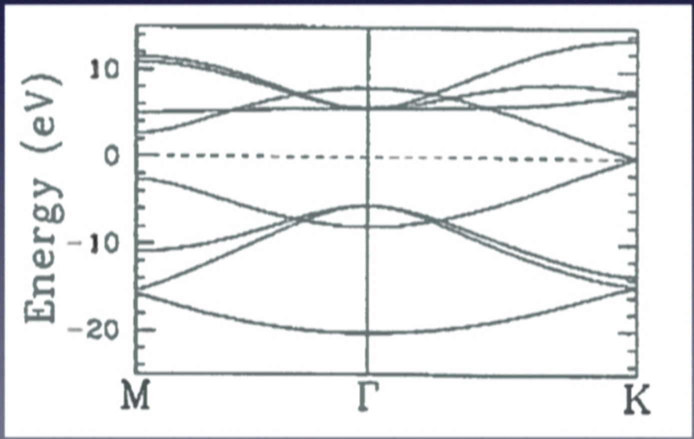

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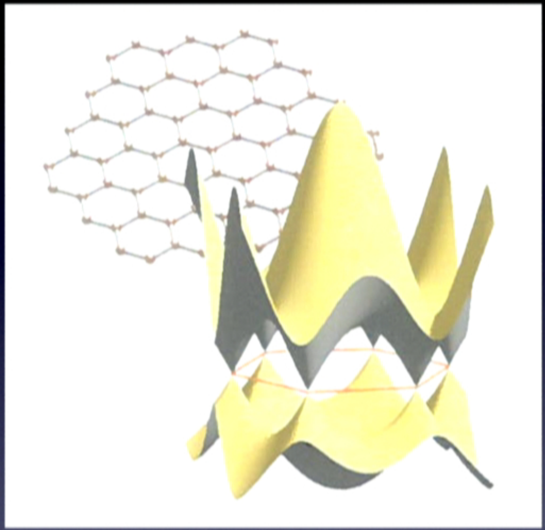

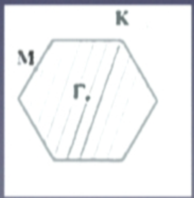

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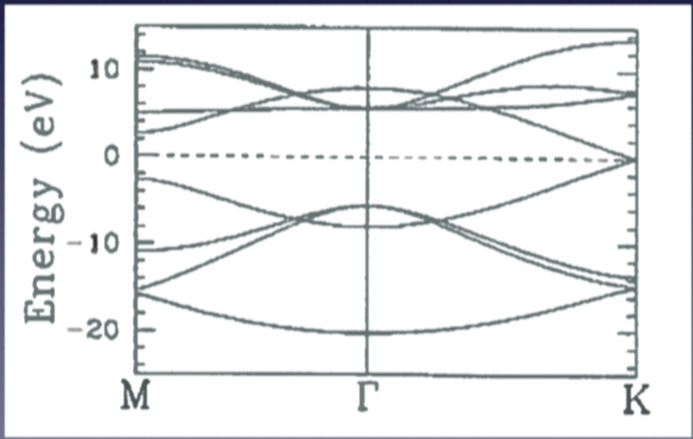
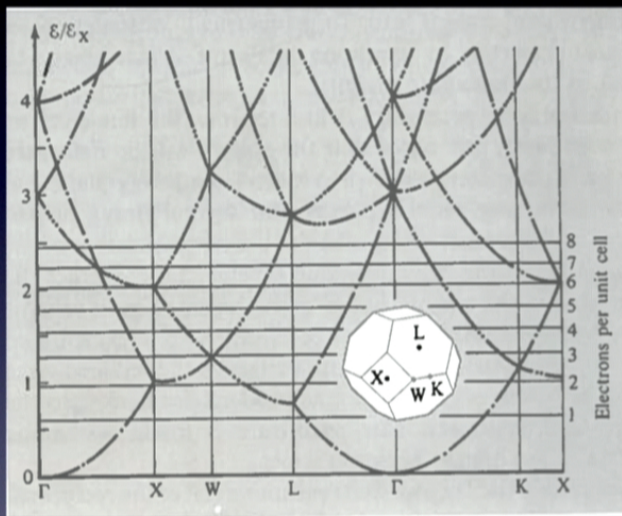


3D band structures



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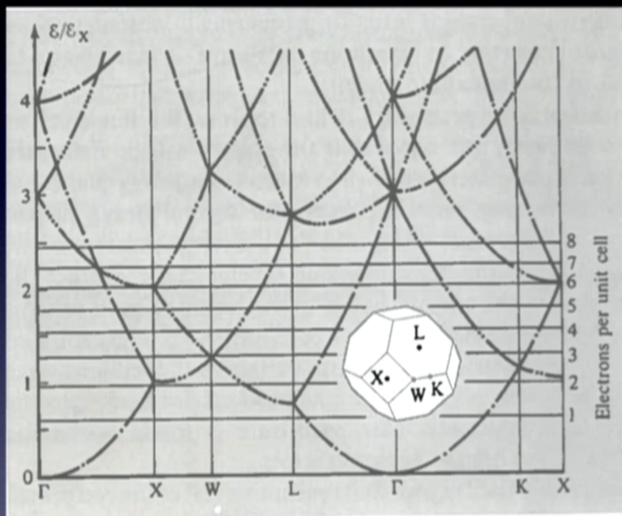
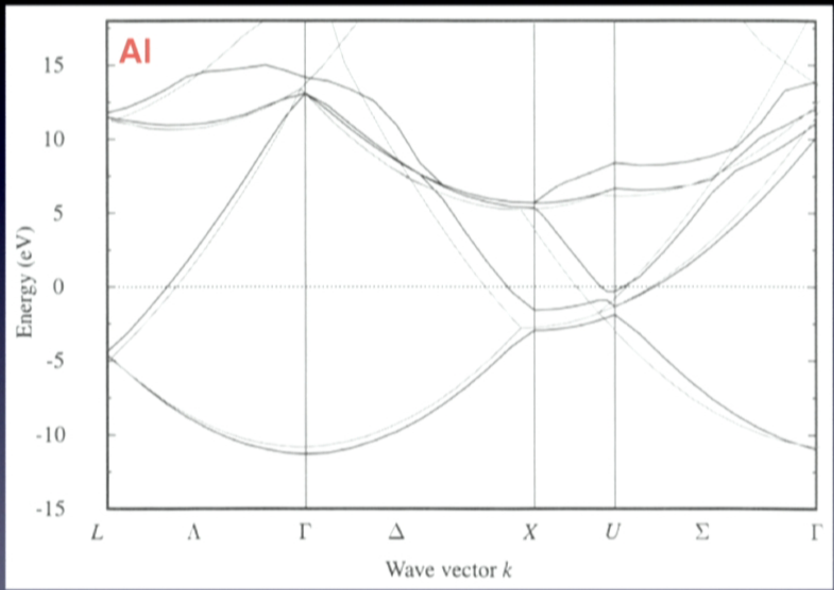


bands for an fcc lattice (zero potential)



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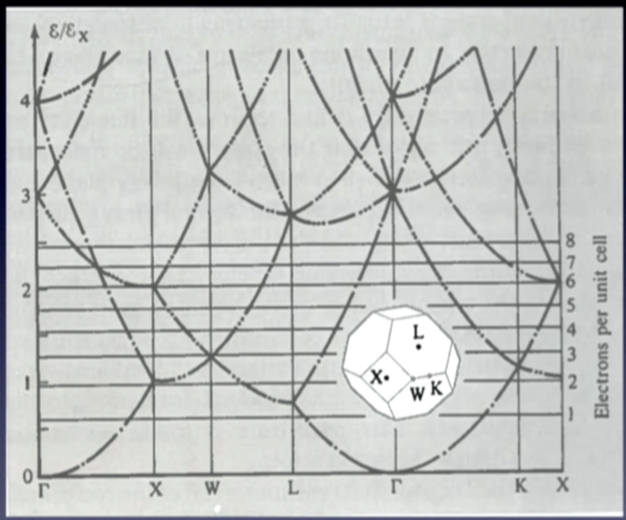

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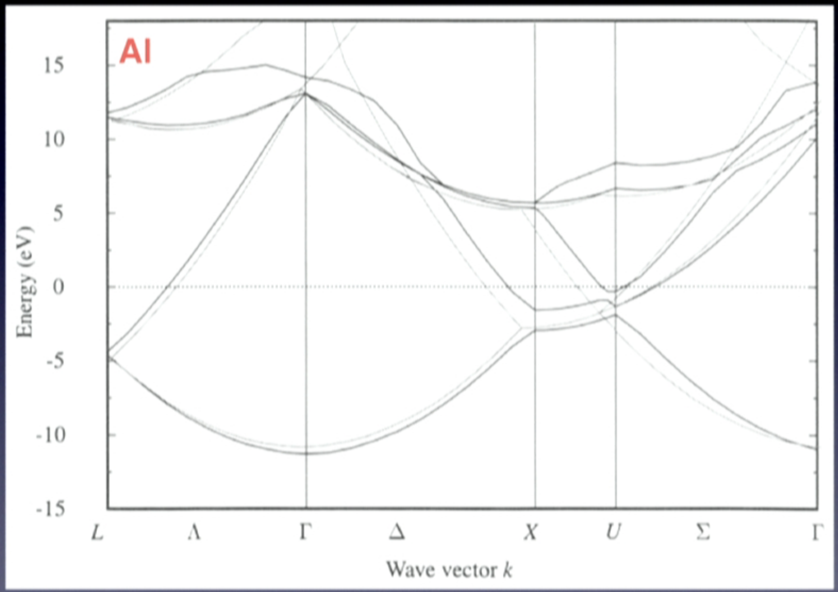

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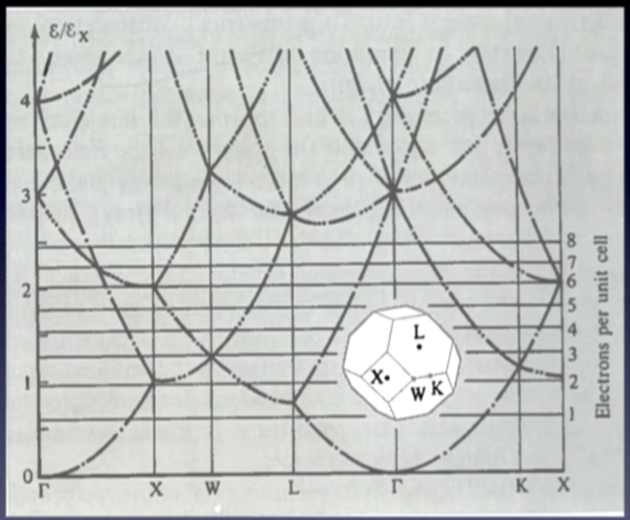

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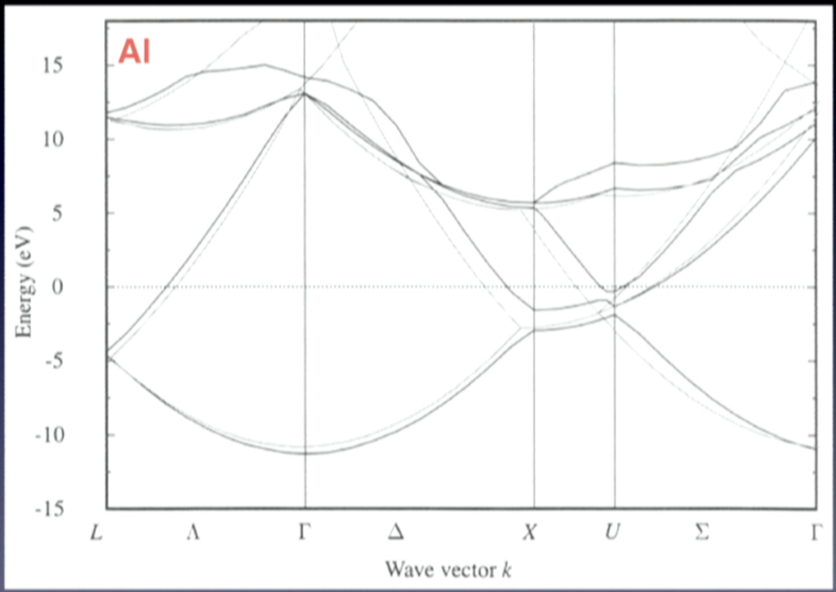
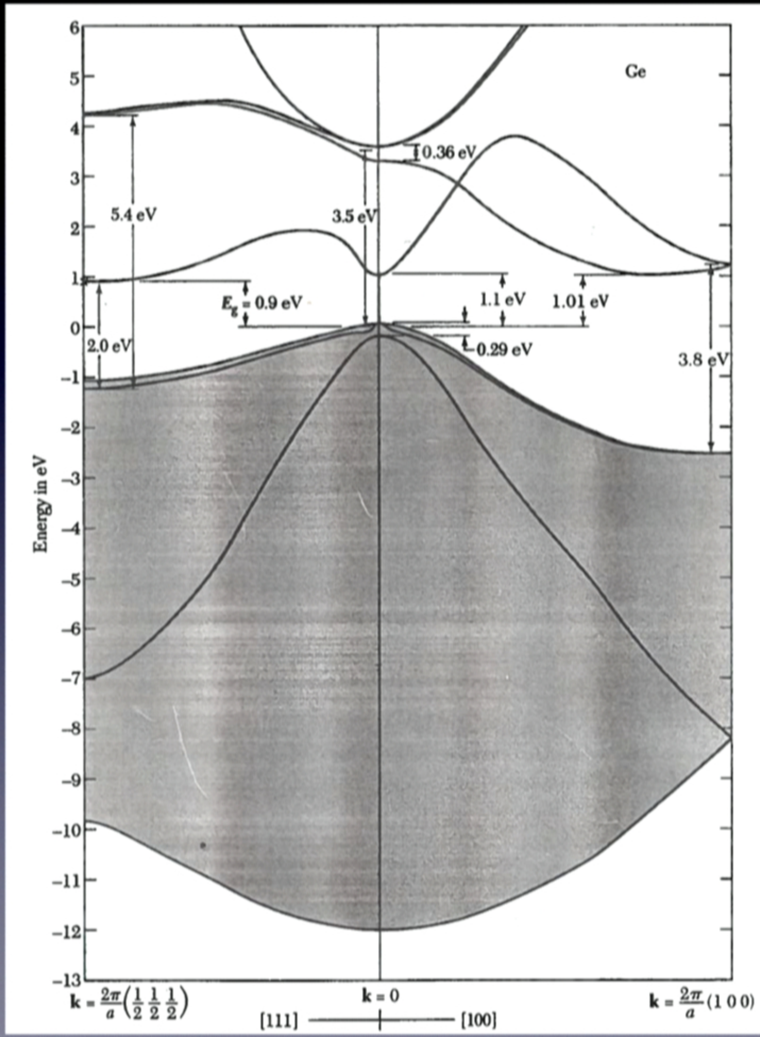


BAND STRUCTURE OF GERMANIUM



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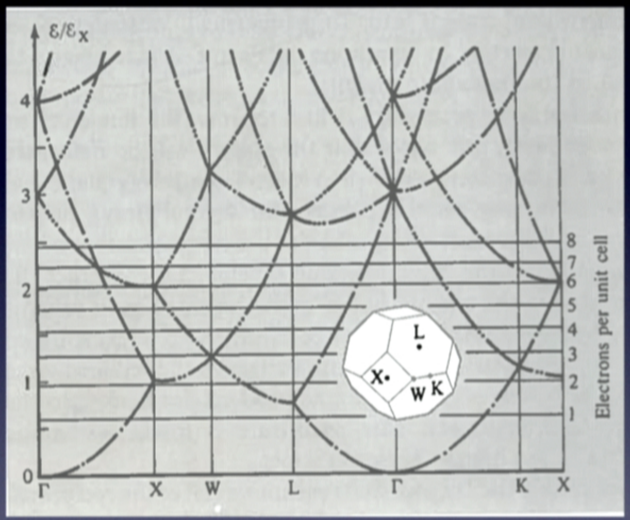

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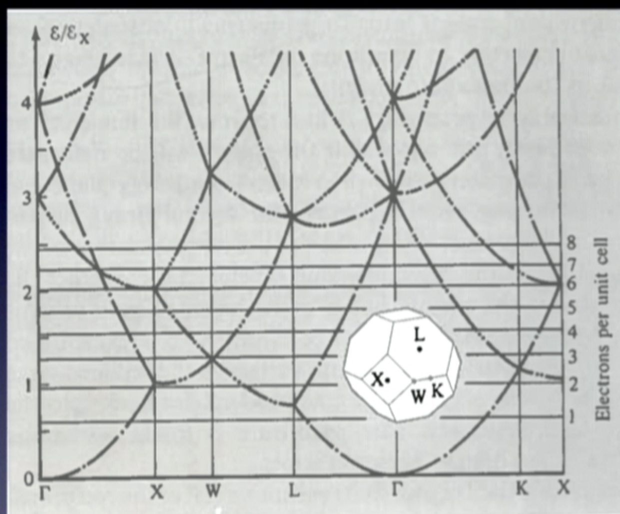

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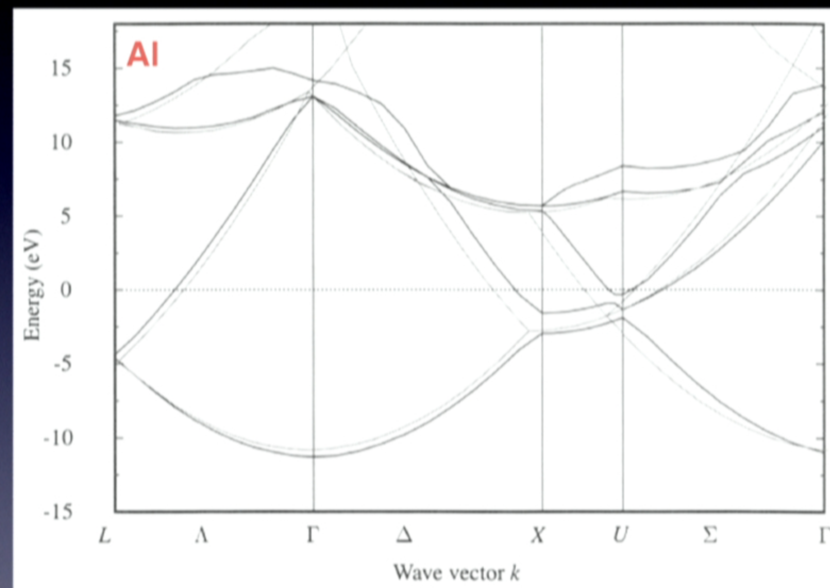

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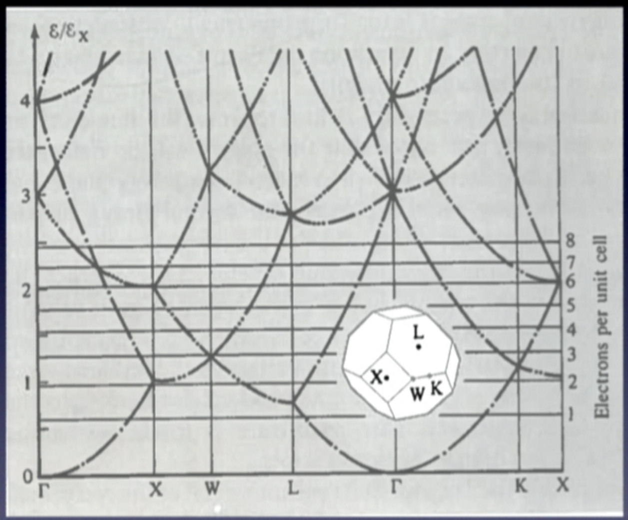

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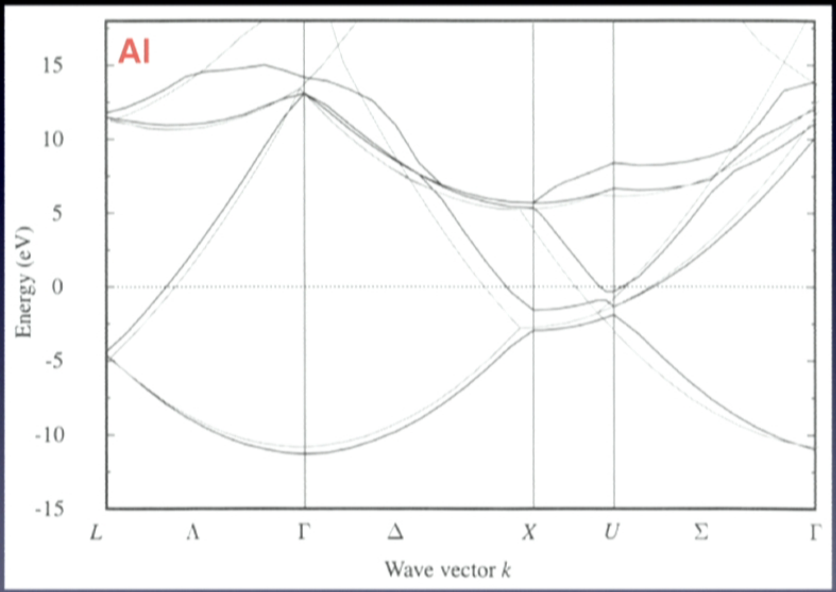

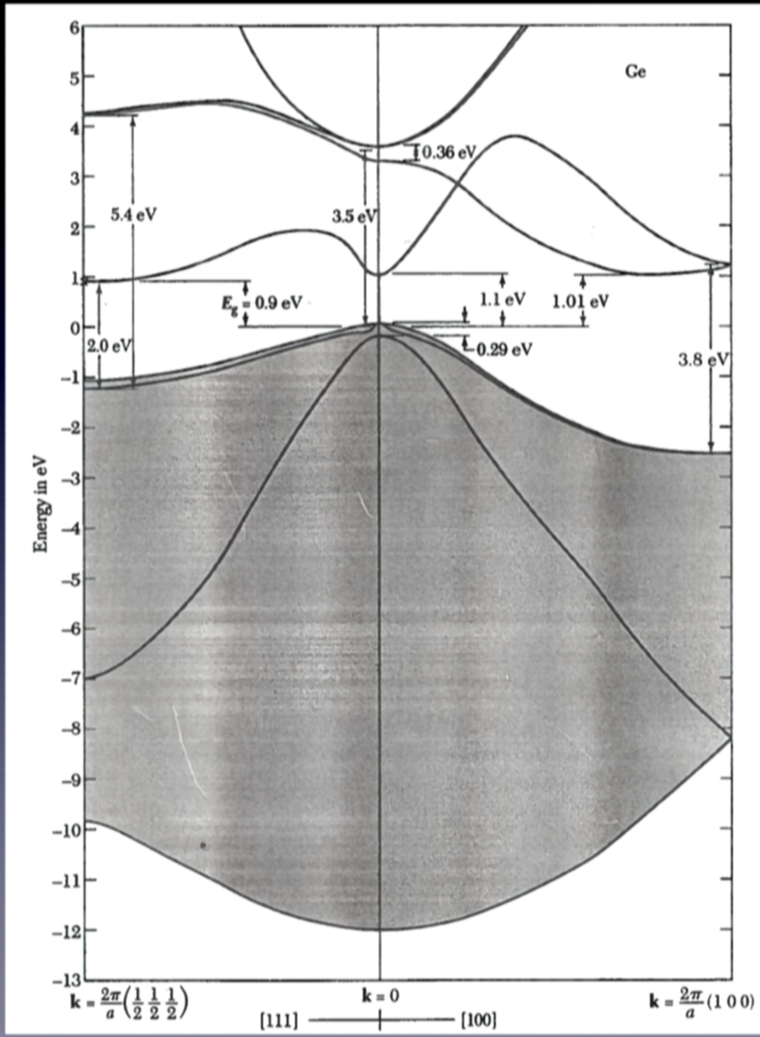

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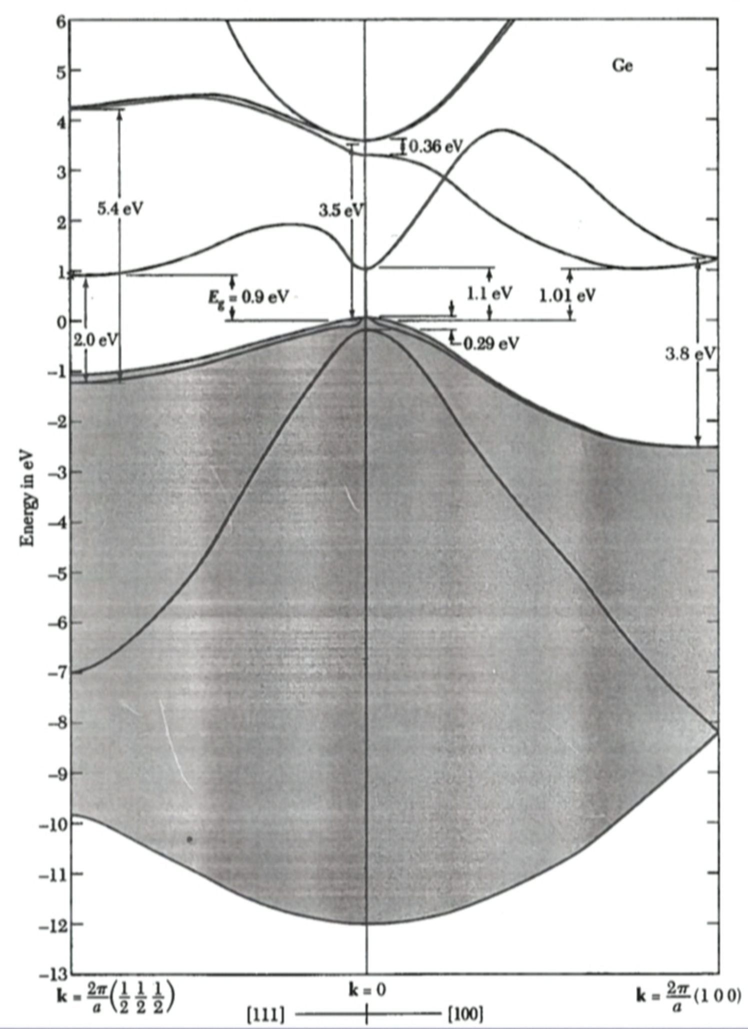

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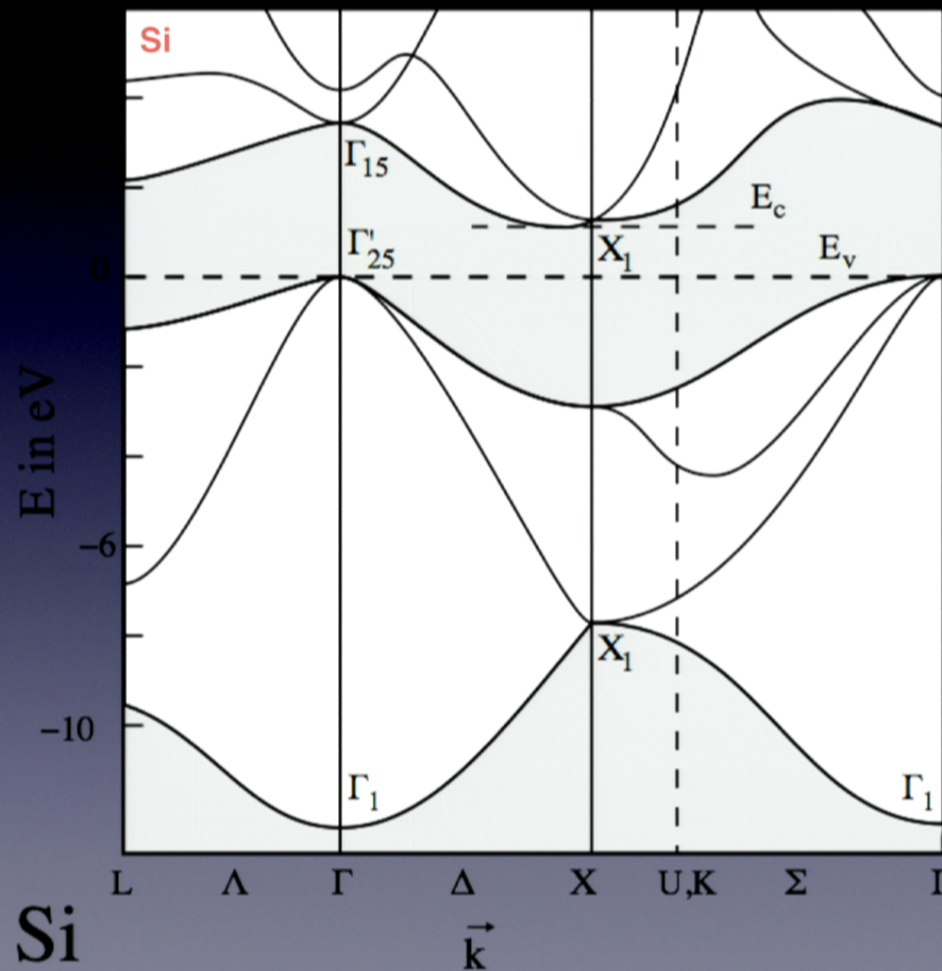
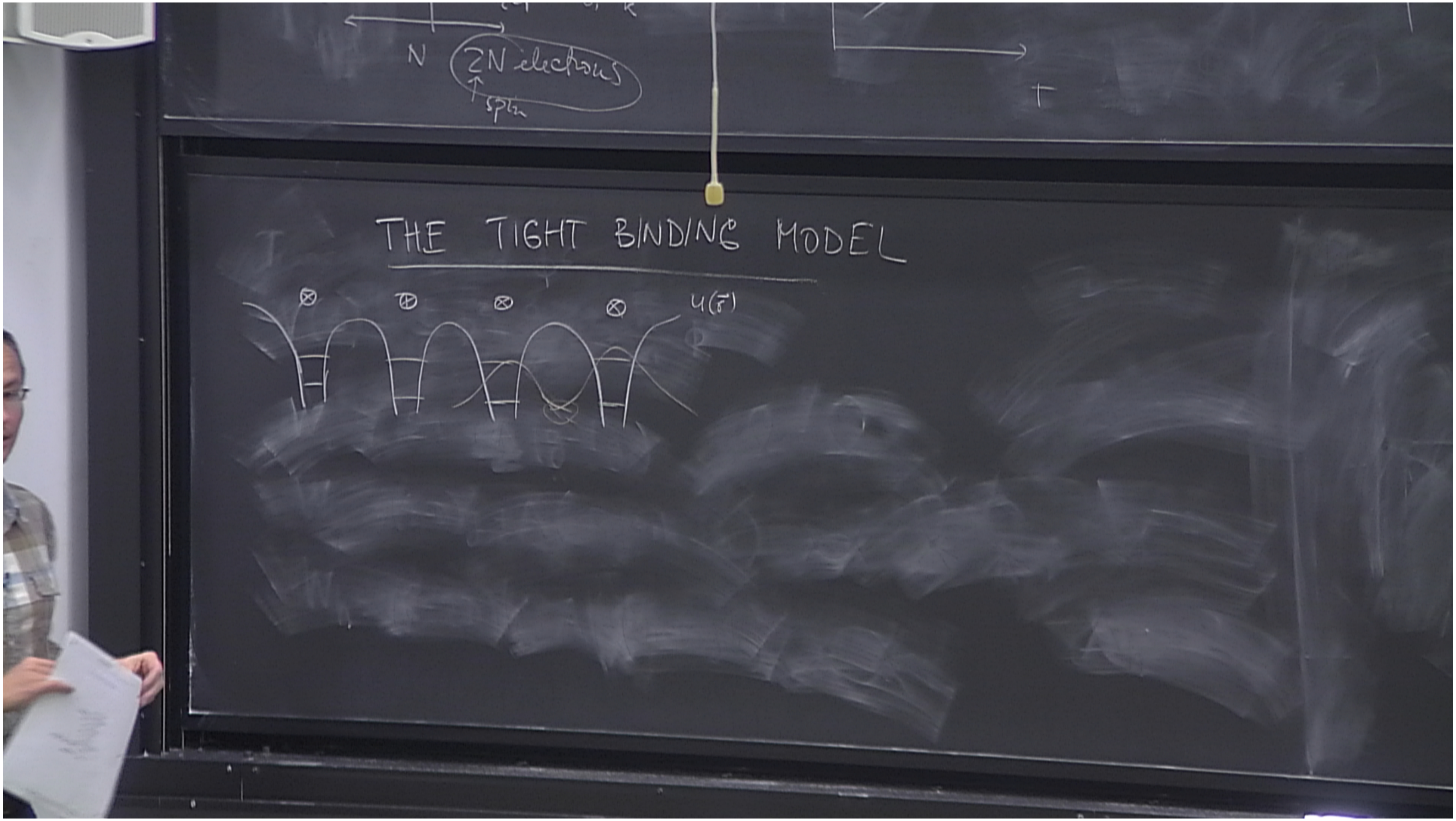
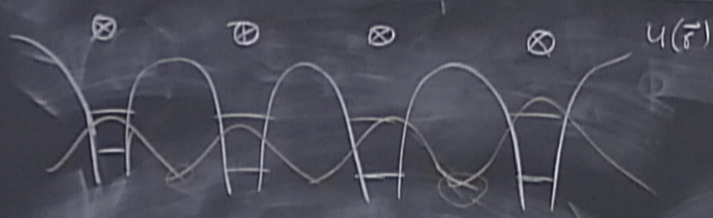

Si
Γ_{15}
Γ'_{25}
X_1
E_c
E_v
0
E in eV
−6
−10
X_1
Γ_1
Γ_1
L Λ Γ Δ X U,K Σ Γ
Si
$\vec{k}$


N
2N electrons
spin
THE TIGHT BINDING MODEL

N 2N electrons

spin

THE TIGHT BINDING MODEL



- treat wf overlaps as small perturbation

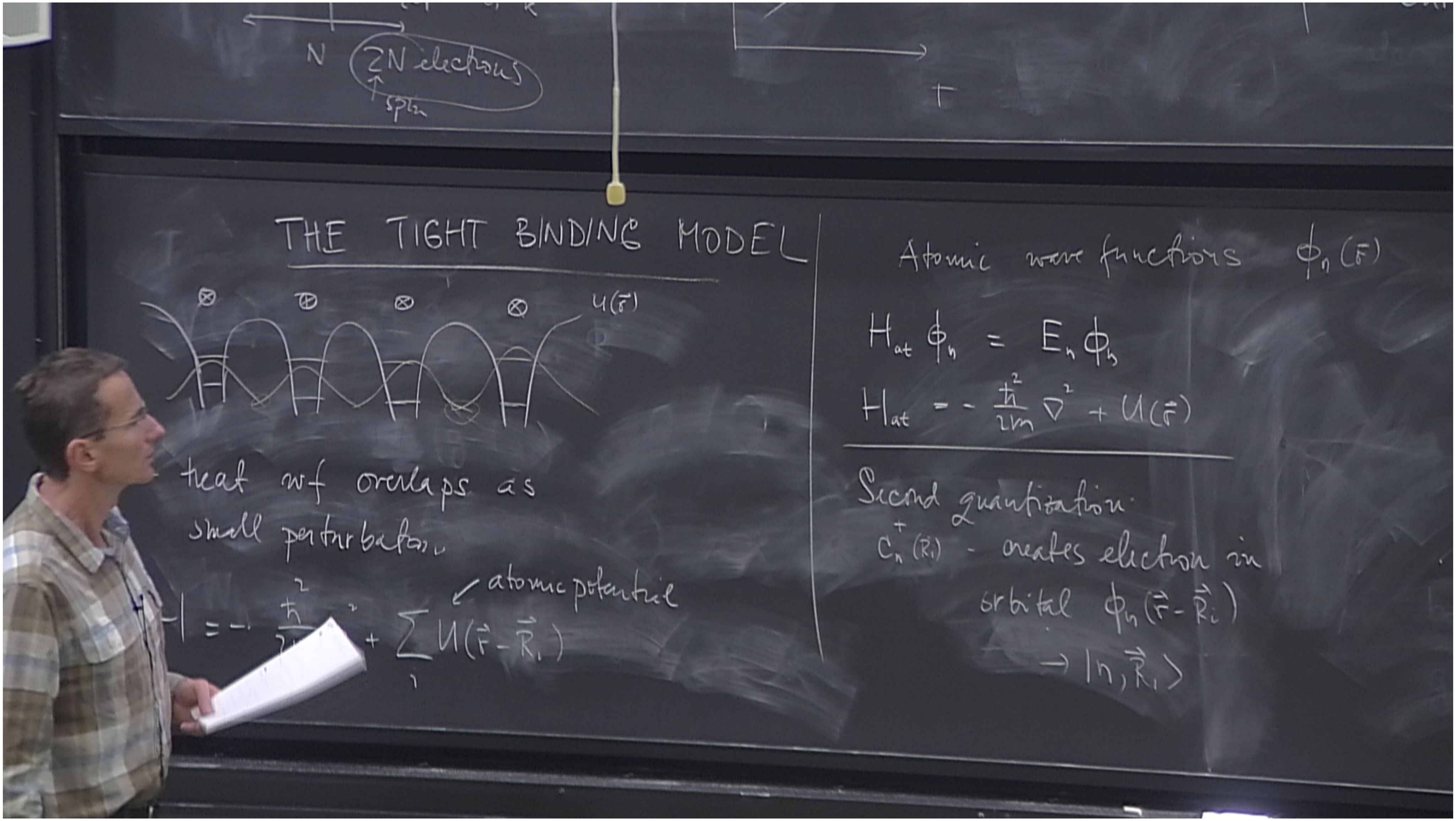
atomic potential

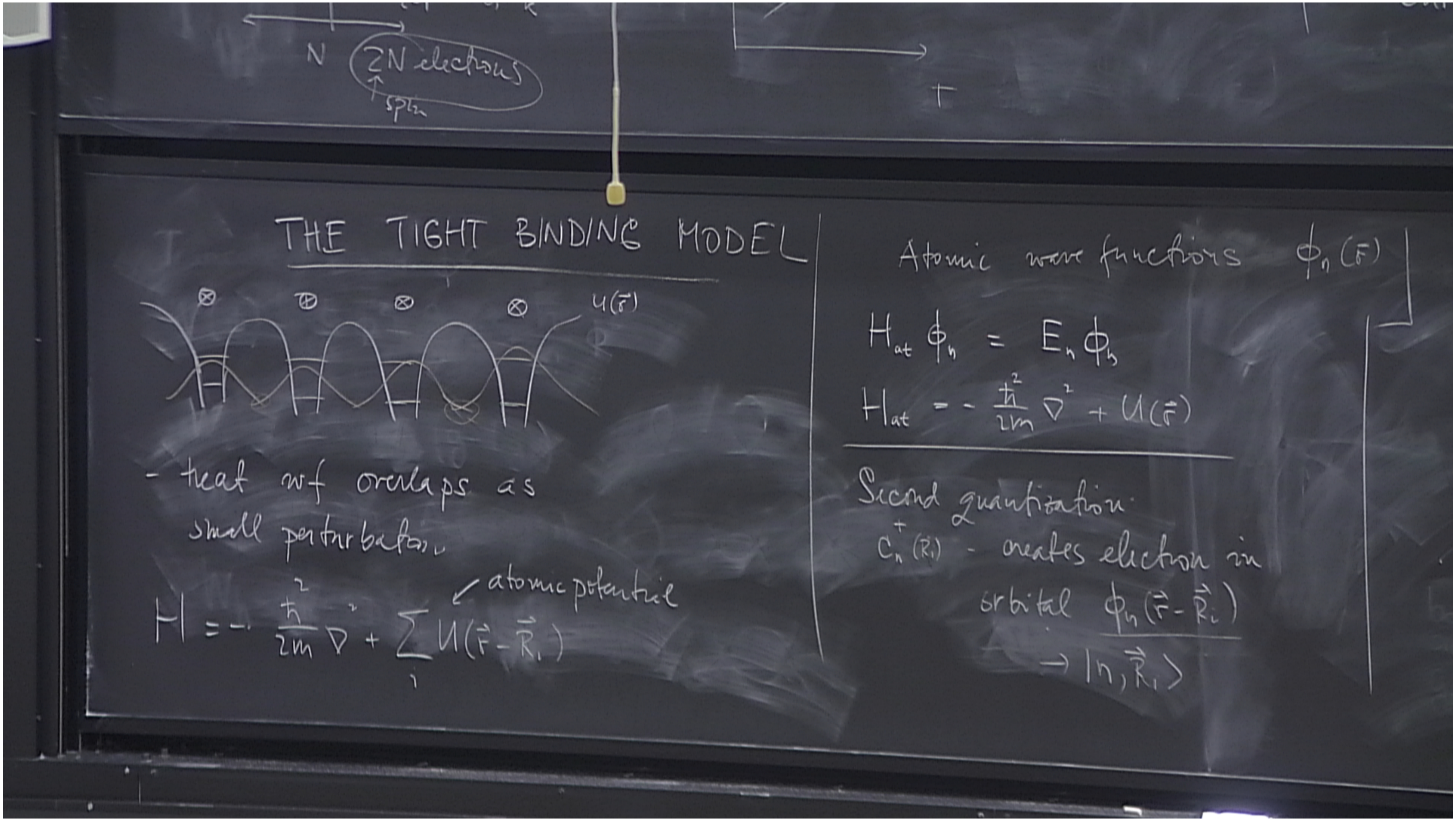
$$H = -\frac{\hbar^2}{2m}\nabla^2 + \sum_i U(\vec{r}-\vec{R}_i)$$

Atomic wave functions $\phi_n(\vec{r})$

$$H_{at}\,\phi_n = E_n\,\phi_n$$

$$H_{at} = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})$$


N
2N electrons
spin
THE TIGHT BINDING MODEL
U(r)
treat wf overlaps as
small perturbation
atomic potential
Atomic wave functions φn(r)
Hat φn = En φn
Hat = - ħ²/2m ∇² + U(r)
Second quantization:
c†n(Ri) - creates electron in
orbital φn(r - Ri)
→ |n, Ri⟩


N
2N electrons
spin
THE TIGHT BINDING MODEL
U(r)
- treat wf overlaps as
small perturbation
atomic potential
H = - ħ²/2m ∇² + Σ_i U(r - R_i)
Atomic wave functions φ_n(r)
H_at φ_n = E_n φ_n
H_at = - ħ²/2m ∇² + U(r)
Second quantization:
c_n^+(R_i) - creates electron in
orbital φ_n(r - R_i)
→ |n, R_i⟩

$$\hat{H} = \sum_{n,m} \sum_{i,j} \langle n, \vec{R}_i | H | m, \vec{R}_j \rangle \, c_n^{\dagger}(\vec{R}_i) \, c_m(\vec{R}_j)$$

- tight-binding Hamiltonian in general form.

...tions $\phi_n(\vec{r})$

$(\vec{r})$

...tion in

$(\vec{r} - \vec{R}_i) \rightarrow \tilde{\phi}_n(\vec{r} - \vec{R}_i)$

$\rangle$

filled bands (weak field cannot produce current)

functions $\phi_n(\vec{r})$

ϕ_3

$+ U(\vec{r})$

on

electron in

$\phi_n(\vec{r}-\vec{R}_i) \to \tilde{\phi}_n(\vec{r}_i-\vec{R}_i)$

$|n, \vec{R}_i\rangle$

$$\hat{H} = \sum_{n,m} \sum_{i,j} \langle n, \vec{R}_i | H | m, \vec{R}_j \rangle \, c_n^\dagger(\vec{R}_i)\, c_m(\vec{R}_j)$$

- tight-binding Hamiltonian in general form.

1) Only wf's on nearby sites have appreciable overlaps.

filled bands (weak field cannot produce current)

functions $\phi_n(\vec{r})$

ϕ_3

$+ U(\vec{r})$

on

electron in

$\phi_n(\vec{r}-\vec{R}_i) \to \tilde{\phi}_n(\vec{r}-\vec{R}_i)$

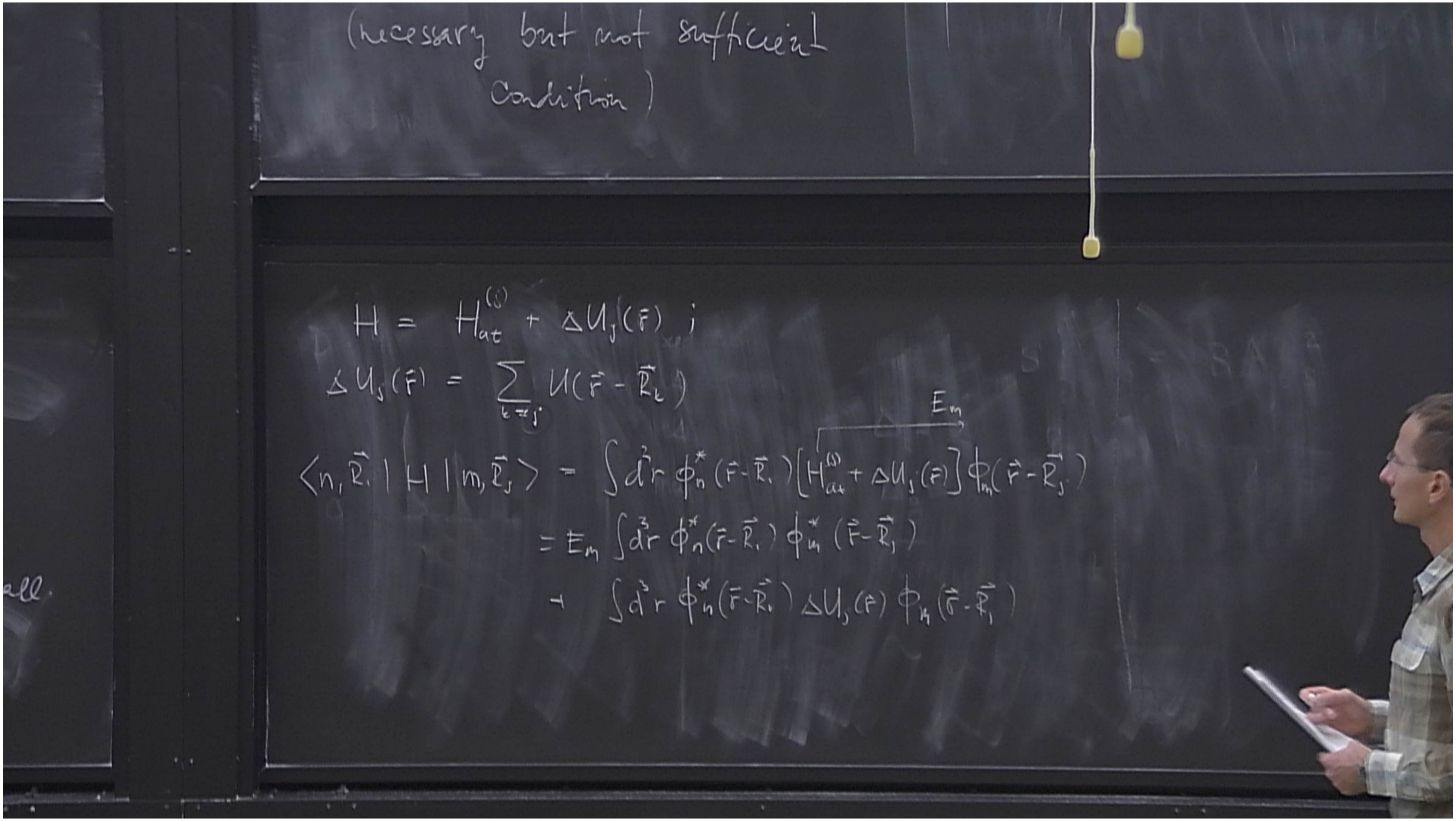
$|n, \vec{R}_i\rangle$

$$\hat{H} = \sum_{n,m} \sum_{i,j} \langle n, \vec{R}_i | H | m, \vec{R}_j \rangle \, c^+_n(\vec{R}_i) \, c_m(\vec{R}_j)$$

- tight-binding Hamiltonian in general form.

1) Only wf's on nearby sites have appreciable overlaps.

2) Wf's for different atomic orbitals (ie $n \neq m$) have different symmetries and therefore again overlap is small.


(necessary but not sufficient condition)
$H = H_{at}^{(j)} + \Delta U_j(\vec{r})$;
$\Delta U_j(\vec{r}) = \sum_{k \neq j} U(\vec{r} - \vec{R}_k)$
E_m
$\langle n, \vec{R}_i | H | m, \vec{R}_j \rangle = \int d^3r \, \phi_n^*(\vec{r} - \vec{R}_i) [H_{at}^{(j)} + \Delta U_j(\vec{r})] \phi_m(\vec{r} - \vec{R}_j)$
$= E_m \int d^3r \, \phi_n^*(\vec{r} - \vec{R}_i) \phi_m(\vec{r} - \vec{R}_j)$
$+ \int d^3r \, \phi_n^*(\vec{r} - \vec{R}_i) \Delta U_j(\vec{r}) \phi_m(\vec{r} - \vec{R}_j)$
all

$$H = H_{at}^{(j)} + \Delta U_j(\vec{r}) \; ;$$

$$\Delta U_j(\vec{r}) = \sum_{k \neq j} U(\vec{r} - \vec{R}_k)$$

$$\langle n, \vec{R}_i \,|\, H \,|\, m, \vec{R}_j \rangle = \int d^3r \, \phi_n^*(\vec{r} - \vec{R}_i) \big[\overbrace{H_{at}^{(j)}}^{E_m} + \Delta U_j(\vec{r}) \big] \phi_m(\vec{r} - \vec{R}_j)$$

$$= E_m \int d^3r \, \phi_n^*(\vec{r} - \vec{R}_i) \, \phi_m^*(\vec{r} - \vec{R}_j)$$

$$+ \int d^3r \, \phi_n^*(\vec{r} - \vec{R}_i) \, \Delta U_j(\vec{r}) \, \phi_m(\vec{r} - \vec{R}_j)$$

$i =$

$\rightarrow$

$\underline{i = j}$

$$\rightarrow \underline{E}_m \delta_{nm} + \overbrace{\int d^3r\, \phi_n^*(\vec{r})\, \Delta U(\vec{r})\, \phi_m(\vec{r})}^{\text{small}}$$

$\underline{E_m}$

$(\vec{r})] \phi_m(\vec{r} - \vec{R}_j)$

$\underline{i \neq j}$

$$\rightarrow \simeq \delta_{nm} t_{ij}, \quad t_{ij} \sim e^{-|\vec{R}_i - \vec{R}_j|/a_0}$$

$\phi_m(\vec{r} - \vec{R}_i)$

E_m

$(\vec{r})]\,\phi_m(\vec{r}-\vec{R}_j)$

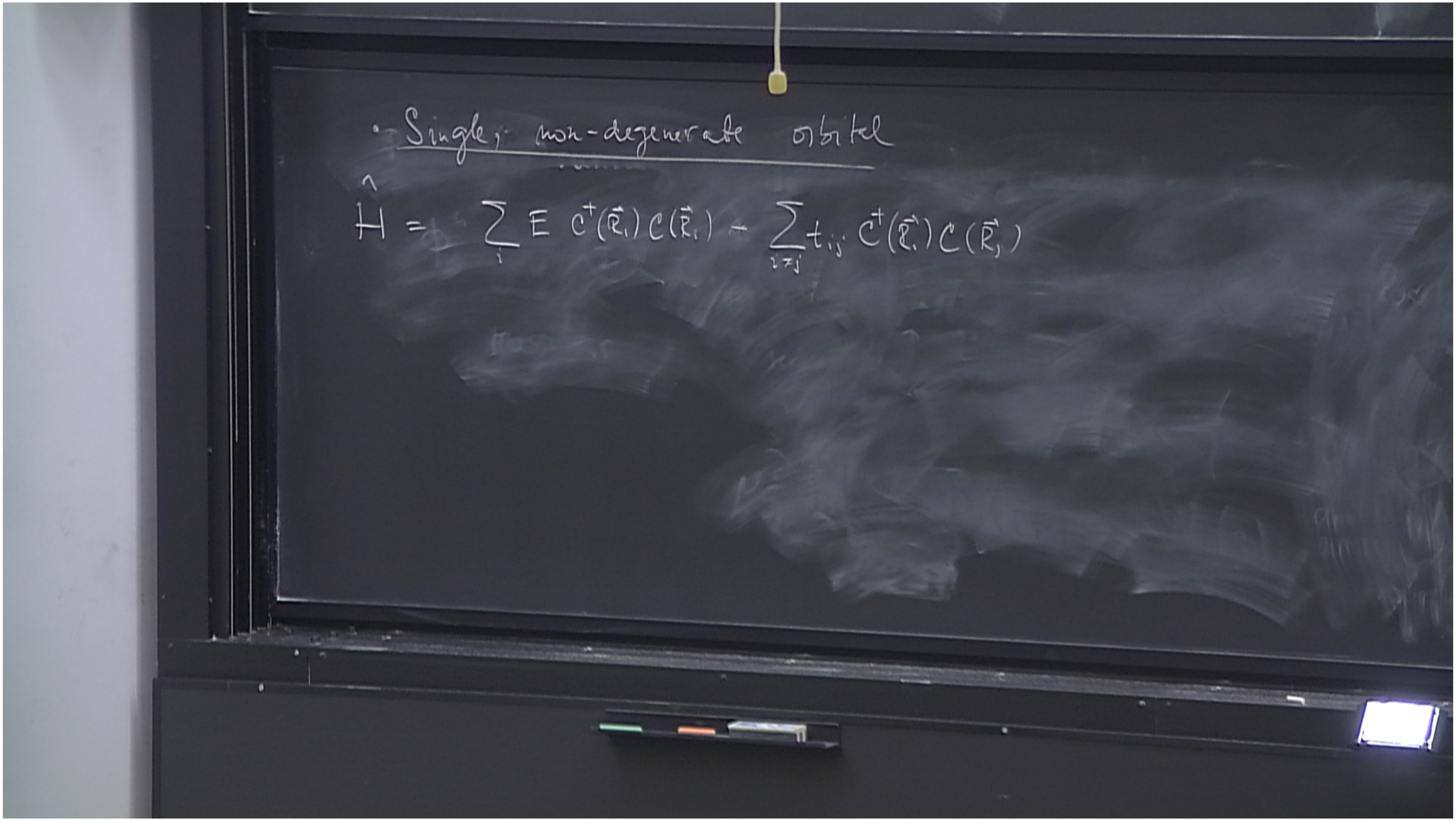
$\phi_n(\vec{r}-\vec{R}_i)$

$\underline{i = j}$

$$\rightarrow \quad \underline{E}_m\,\delta_{nm} + \overbrace{\int d^3r\, \phi_n^*(\vec{r})\, \Delta U(\vec{r})\, \phi_m(\vec{r})}^{\text{small}}$$

$\underline{i \neq j}$

$$\rightarrow \quad \simeq \underline{\delta_{nm}\, t_{ij}}\,, \qquad t_{ij} \sim e^{-|\vec{R}_i - \vec{R}_j|/a_0}$$


• Single, non-degenerate orbital
$\hat{H} = \sum_i E\, c^\dagger(\vec{R}_i)\, c(\vec{R}_i) - \sum_{i \neq j} t_{ij}\, c^\dagger(\vec{R}_i)\, c(\vec{R}_j)$

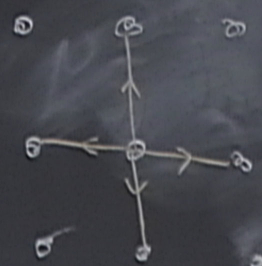
- Single, non-degenerate orbital

$$\hat{H} = \sum_i E_0 \, c^\dagger(\vec{R}_i)\, c(\vec{R}_i) + \sum_{i \neq j} t_{ij}\, c^\dagger(\vec{R}_i)\, c(\vec{R}_j)$$

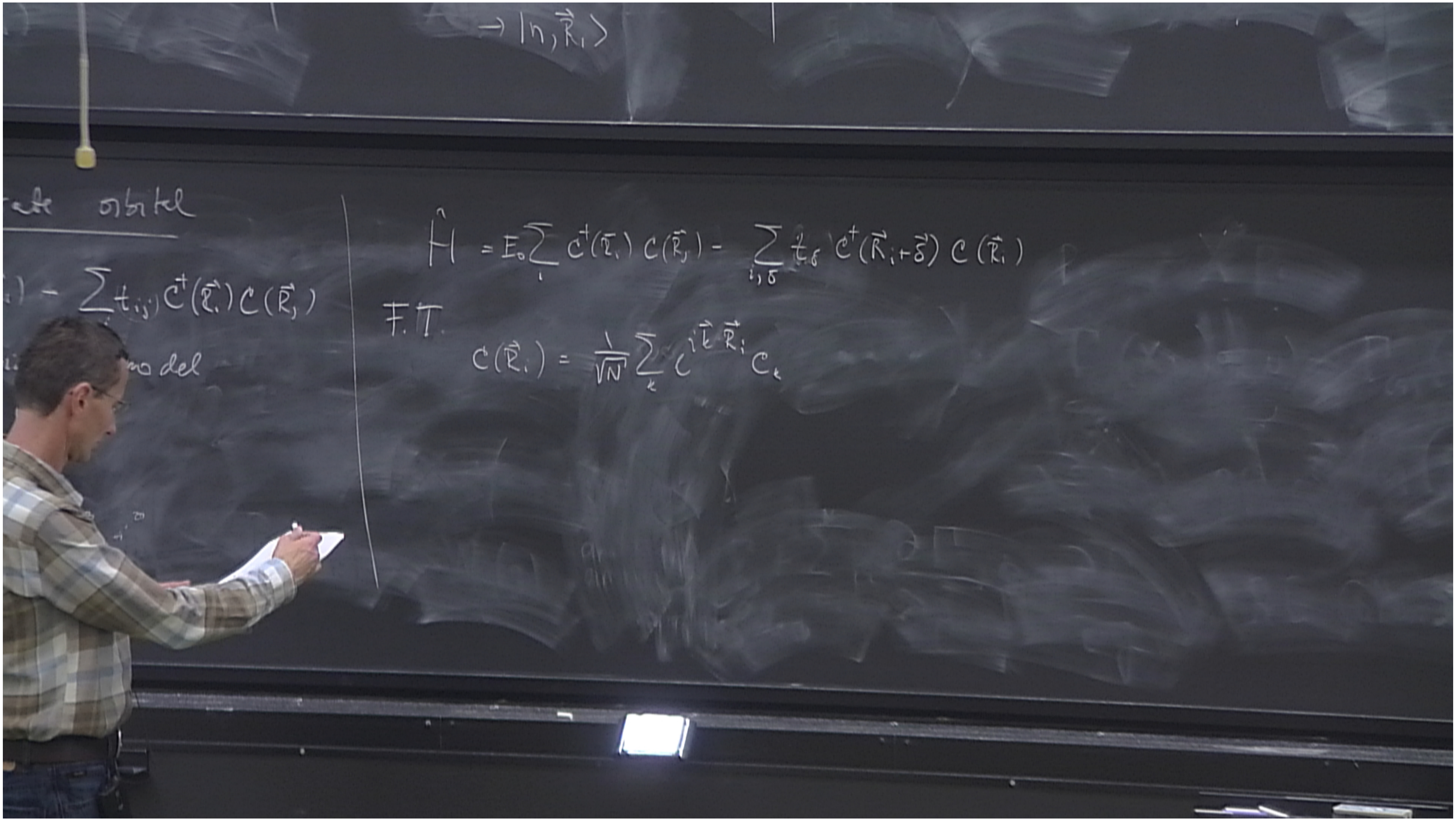
- nearest-neighbor tight-binding model

$$t_{ij} = \begin{cases} t, & \vec{R}_i, \vec{R}_j \in \text{n.n.} \\ 0, & \text{otherwise} \end{cases}$$

- square lattice in 2D



$\hat{H} =$


$\rightarrow |n, \vec{R}_i\rangle$
orbital
$\hat{H} = E_0 \sum_i c^\dagger(\vec{R}_i)\, c(\vec{R}_i) - \sum_{i,\delta} t_\delta\, c^\dagger(\vec{R}_i + \vec{\delta})\, c(\vec{R}_i)$
$- \sum t_{ij}\, c^\dagger(\vec{R}_i)\, c(\vec{R}_j)$
F.T.
$c(\vec{R}_i) = \frac{1}{\sqrt{N}} \sum_k e^{i\vec{k}\cdot\vec{R}_i} c_k$
model

$\to |n, \vec{R}_i\rangle$

...ate orbital

$\ldots) - \sum_{i\neq j} t_{ij}\, c^\dagger(\vec{R}_i)\, c(\vec{R}_j)$

...inding model

n.n.

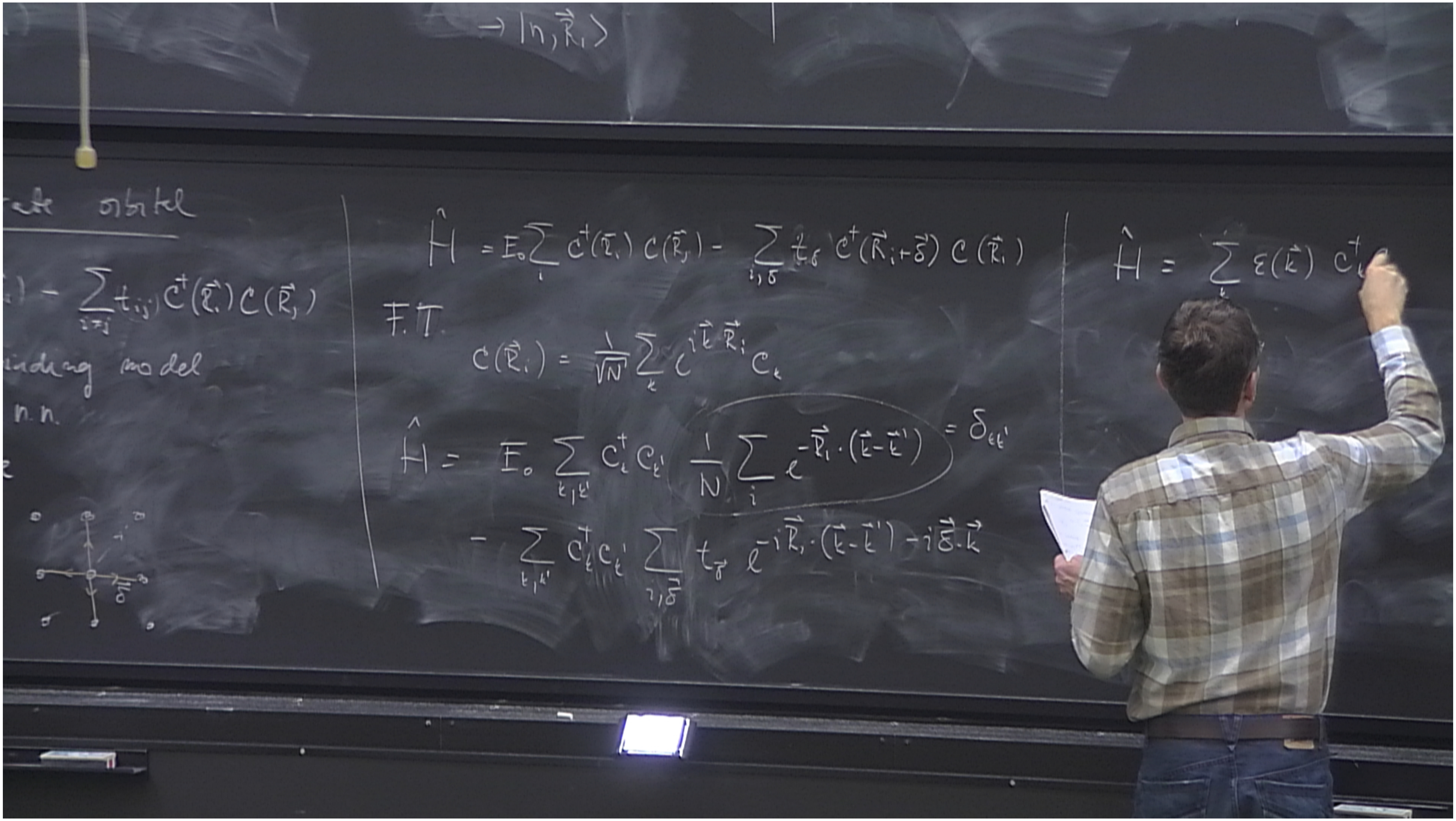
$$\hat{H} = E_0 \sum_i c^\dagger(\vec{R}_i)\, c(\vec{R}_i) - \sum_{i,\delta} t_\delta\, c^\dagger(\vec{R}_i+\vec{\delta})\, c(\vec{R}_i)$$

F.T.

$$c(\vec{R}_i) = \frac{1}{\sqrt{N}} \sum_k e^{i\vec{k}\vec{R}_i} c_k$$

$$\hat{H} = E_0 \sum_{k,k'} c_k^\dagger c_{k'} \frac{1}{N} \sum_i e^{-\vec{R}_i\cdot(\vec{k}-\vec{k}')}$$

$$- \sum_{k,k'} c_k^\dagger c_{k'} \sum_{i,\vec{\delta}} t_\delta\, e^{-i\vec{R}_i\cdot(\vec{k}-\vec{k}') - i\vec{\delta}\cdot\vec{k}}$$



$\hat{H} = E_0 \sum_i c^\dagger(\vec{R}_i)\, c(\vec{R}_i) - \sum_{i,\delta} t_\delta\, c^\dagger(\vec{R}_i + \vec{\delta})\, c(\vec{R}_i)$
F.T.
$c(\vec{R}_i) = \frac{1}{\sqrt{N}} \sum_k e^{i\vec{k}\cdot\vec{R}_i} c_k$
$\hat{H} = E_0 \sum_{k,k'} c_k^\dagger c_{k'} \frac{1}{N} \sum_i e^{-\vec{R}_i\cdot(\vec{k}-\vec{k}')} = \delta_{kk'}$
$- \sum_{k,k'} c_k^\dagger c_{k'} \sum_{i,\vec{\delta}} t_\delta\, e^{-i\vec{R}_i\cdot(\vec{k}-\vec{k}') - i\vec{\delta}\cdot\vec{k}}$
$\hat{H} = \sum_k \varepsilon(\vec{k})\, c_k^\dagger$
$- \sum_{i \neq j} t_{ij}\, c^\dagger(\vec{R}_i)\, c(\vec{R}_j)$
model
n.n.
$\vec{\delta}$

$$c^\dagger(\vec{r}_i)\, c(\vec{R}_j) - \sum_{i,\delta} t_\delta\, c^\dagger(\vec{R}_i+\vec{\delta})\, c(\vec{R}_i)$$

$$= \frac{1}{\sqrt{N}} \sum_k e^{i\vec{k}\cdot\vec{R}_i}\, c_k$$

$$\sum_{k,k'} c_k^\dagger c_{k'}\, \frac{1}{N}\sum_i e^{-\vec{R}_i\cdot(\vec{k}-\vec{k}')} = \delta_{kk'}$$

$$c_k^\dagger c_{k'} \sum_{i,\vec{\delta}} t_{\vec{\delta}}\, e^{-i\vec{R}_i\cdot(\vec{k}-\vec{k}') - i\vec{\delta}\cdot\vec{k}}$$

$$\boxed{\begin{aligned} \hat{H} &= \sum_k \varepsilon(\vec{k})\, c_k^\dagger c_k \\ \varepsilon(\vec{k}) &= E_0 - \sum_{\vec{\delta}} t_{\vec{\delta}}\, e^{-i\vec{k}\cdot\vec{\delta}} \end{aligned}}$$

tight-binding dispersion

$$c^\dagger(\vec{R}_i)\,c(\vec{R}_i) - \sum_{i,\delta} t_\delta\, c^\dagger(\vec{R}_i+\vec{\delta})\, c(\vec{R}_i)$$

$$= \frac{1}{\sqrt{N}} \sum_k e^{i\vec{k}\cdot\vec{R}_i} c_k$$

$$\sum_{k,k'} c_k^\dagger c_{k'} \frac{1}{N}\sum_i e^{-\vec{R}_i\cdot(\vec{k}-\vec{k}')} = \delta_{kk'}$$

$$c_k^\dagger c_{k'} \sum_{i,\vec{\delta}} t_\delta\, e^{-i\vec{R}_i\cdot(\vec{k}-\vec{k}')-i\vec{\delta}\cdot\vec{k}}$$

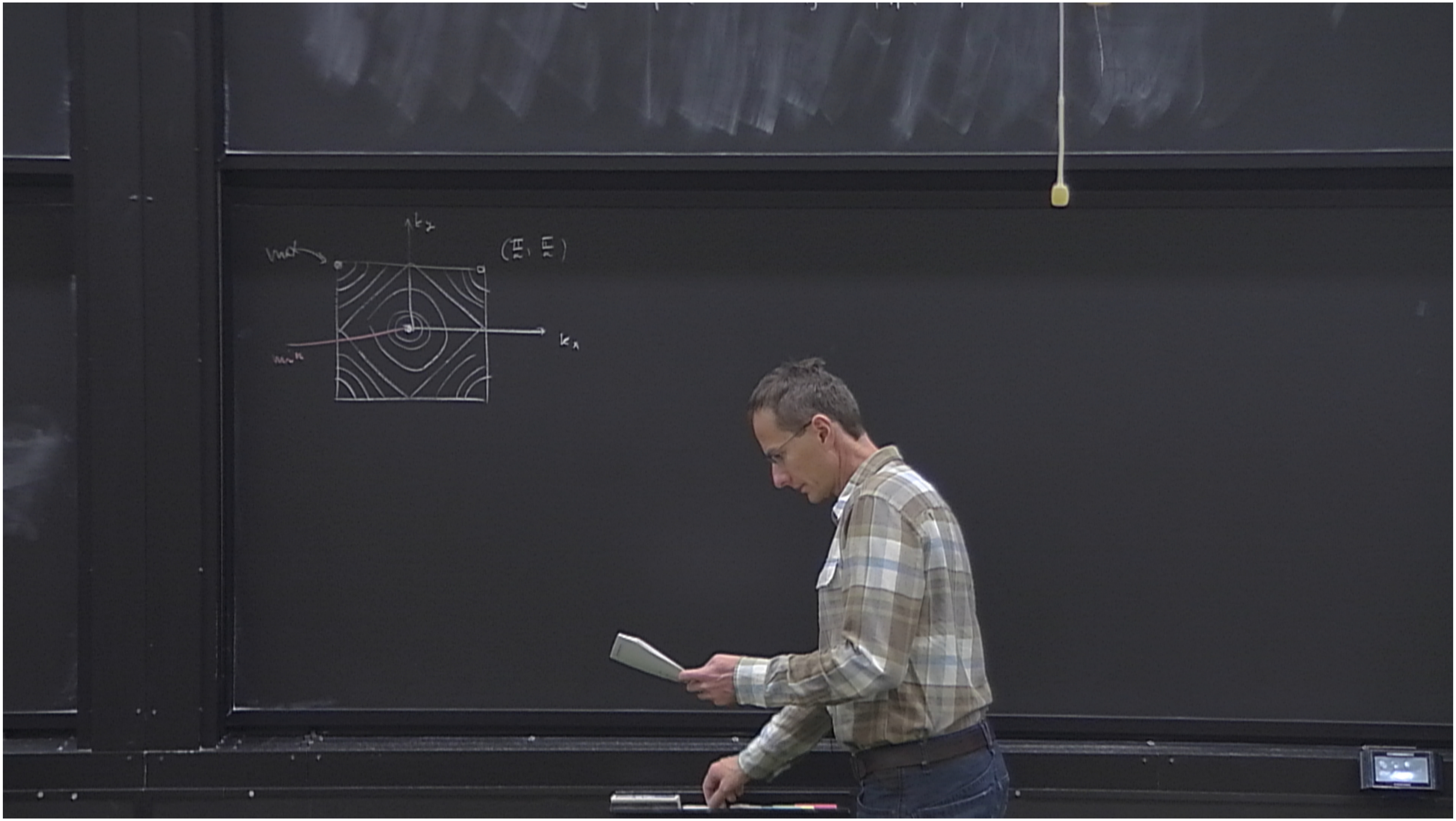
$$\boxed{\begin{aligned}\hat{H} &= \sum_k \varepsilon(\vec{k})\, c_k^\dagger c_k \\ \varepsilon(\vec{k}) &= E_0 - \sum_{\vec{\delta}} t_{\vec{\delta}}\, e^{-i\vec{k}\cdot\vec{\delta}}\end{aligned}}$$

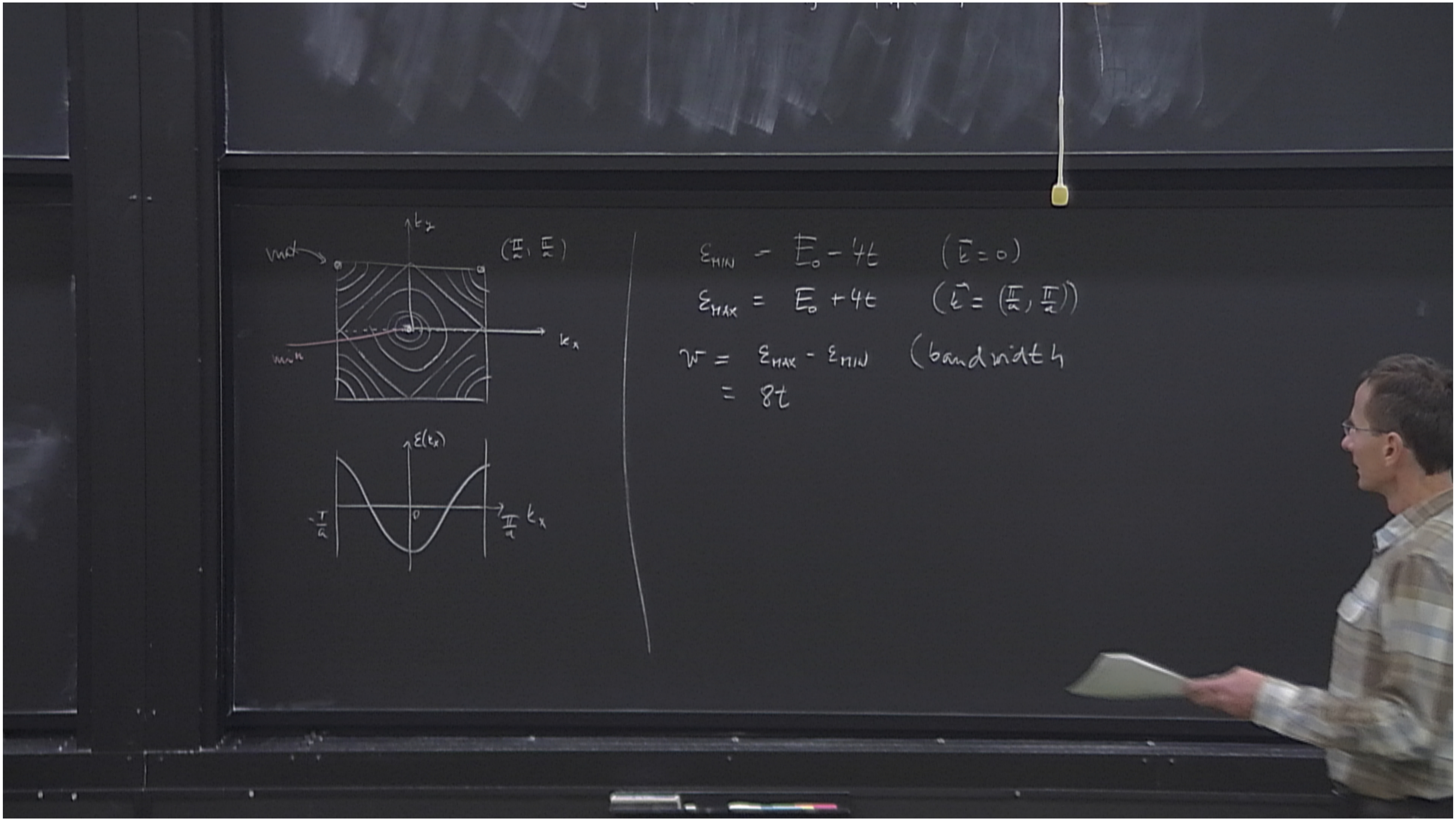
tight-binding dispersion

<u>EXAMPLE</u> n.n, square latt

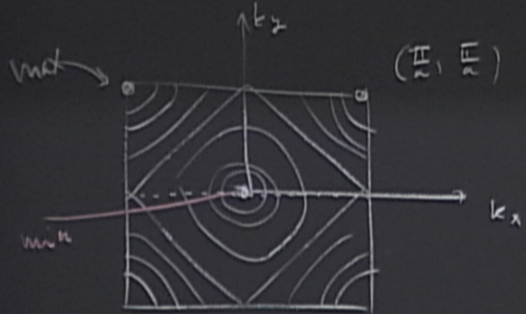
$$\vec{\delta} = (\pm a\hat{x}, \pm a\hat{y}), \quad t_{\vec{\delta}} = t$$

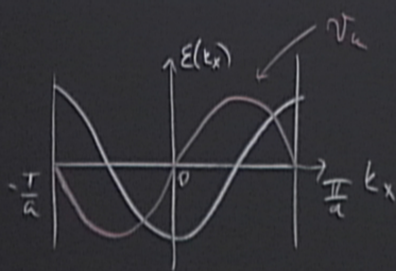
$$\varepsilon(\vec{k}) = E_0 - 2t\left[\cos(ak_x) + \cos(ak_y)\right]$$


max
min
k_y
k_x



k_y
$(\frac{\pi}{a}, \frac{\pi}{a})$
max
min
k_x
$\varepsilon(k_x)$
$-\frac{\pi}{a}$
0
$\frac{\pi}{a}$
k_x
$\varepsilon_{MIN} = E_0 - 4t \quad (\vec{k} = 0)$
$\varepsilon_{MAX} = E_0 + 4t \quad (\vec{k} = (\frac{\pi}{a}, \frac{\pi}{a}))$
$W = \varepsilon_{MAX} - \varepsilon_{MIN}$ (bandwidth
$= 8t$





$\varepsilon_{MIN} = E_0 - 4t \quad (\vec{k} = 0)$

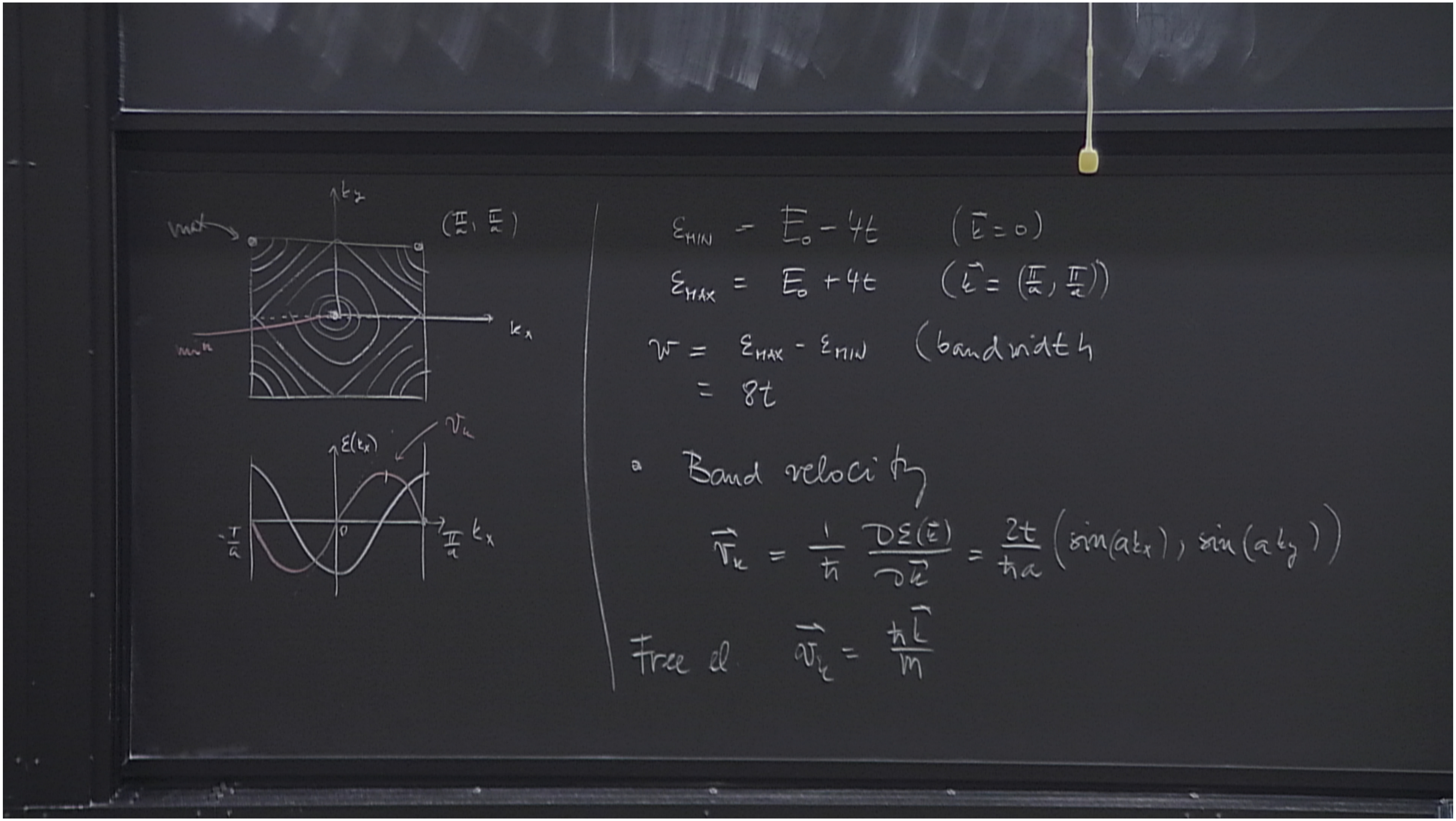
$\varepsilon_{MAX} = E_0 + 4t \quad (\vec{k} = (\frac{\pi}{a}, \frac{\pi}{a}))$

$W = \varepsilon_{MAX} - \varepsilon_{MIN}$ (bandwidth

$= 8t$

- Band velocity

$$\vec{v}_k = \frac{1}{\hbar} \frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}} = \frac{2t}{\hbar a} \left(\sin(a k_x), \sin(a k_y) \right)$$



k_y
max
(π/a, π/a)
k_x
min
ε(k_x)
v_k
-π/a
0
π/a
ε_MIN = E_0 - 4t   (k = 0)
ε_MAX = E_0 + 4t   (k = (π/a, π/a))
W = ε_MAX - ε_MIN   (bandwidth
= 8t
Band velocity
v_k = (1/ħ) ∂ε(k)/∂k = (2t/ħa) (sin(ak_x), sin(ak_y))
Free el.   v_k = ħk/m