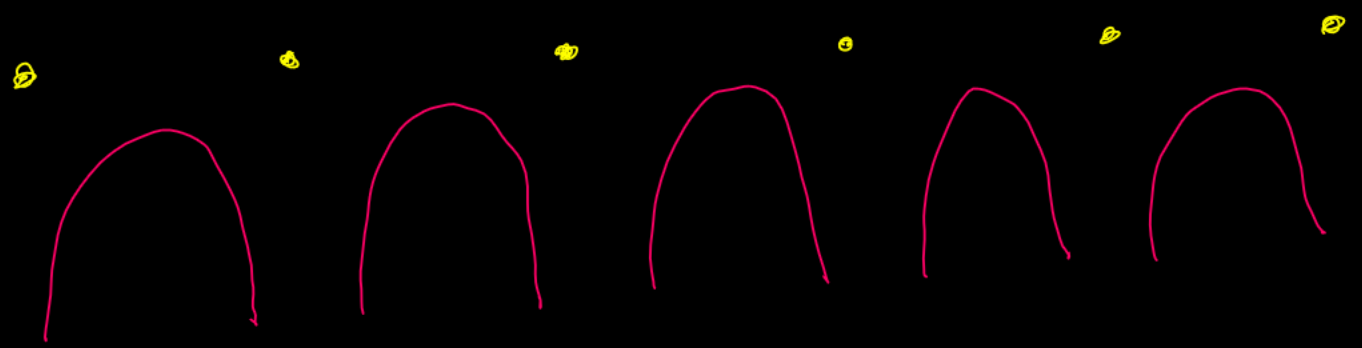
Lecture 12

Wednesday, Feb. 10, 2021

CHAP 7 ELECTRONS IN A PERIODIC POTENTIAL



$$U(\vec{r}) = U(\vec{r} + \vec{R}) \quad \forall \vec{R} \in D.L.$$

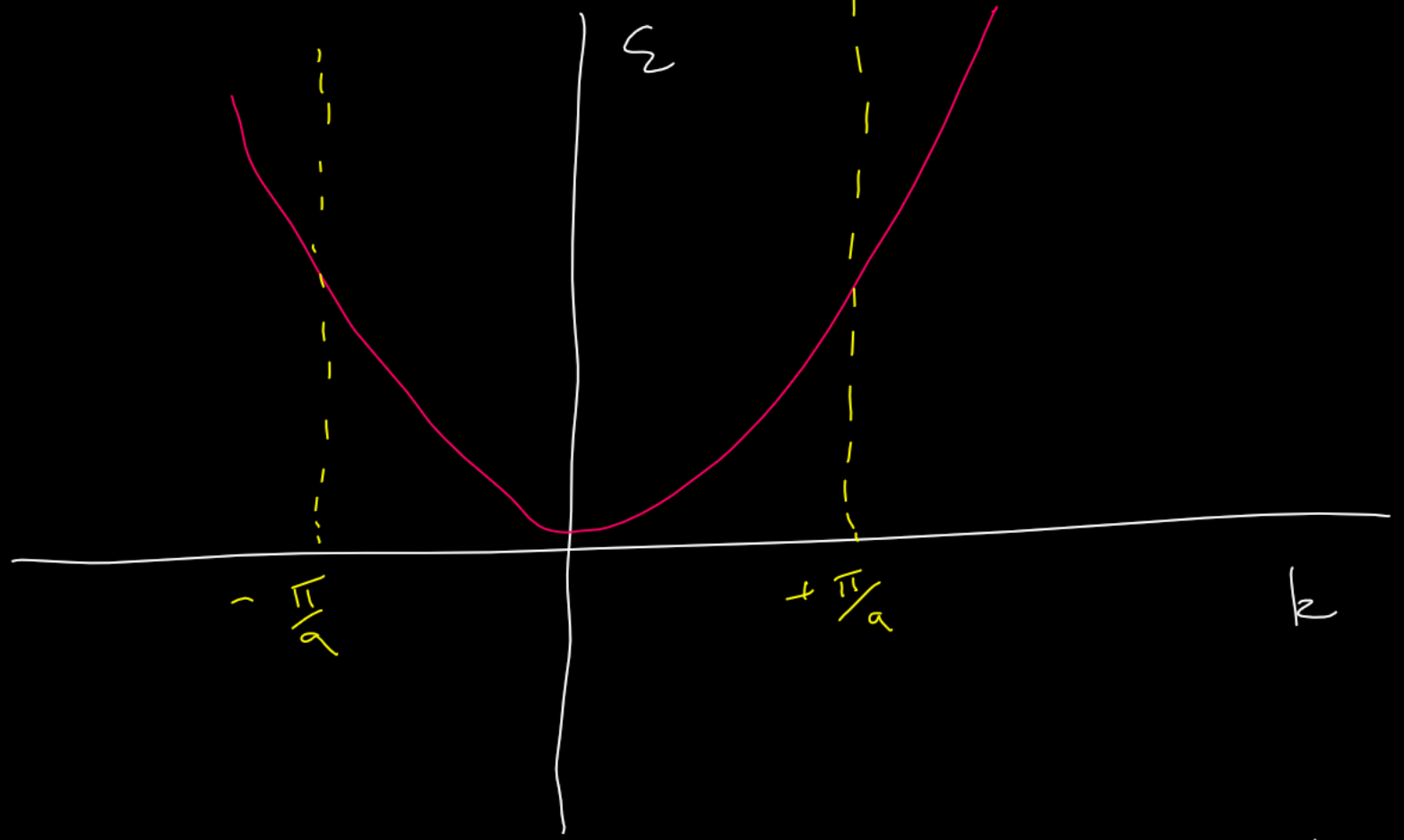
SINGLE ELECTRON $\Rightarrow$ $H = \sum_i H_i$

H_i ← SINGLE ELECTRON

NO LATTICE INTERACTIONS

$$\varepsilon(\vec{k}) = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) \qquad \psi = \frac{1}{\sqrt{V}}\, e^{i\vec{k}\cdot\vec{r}}$$

1-D



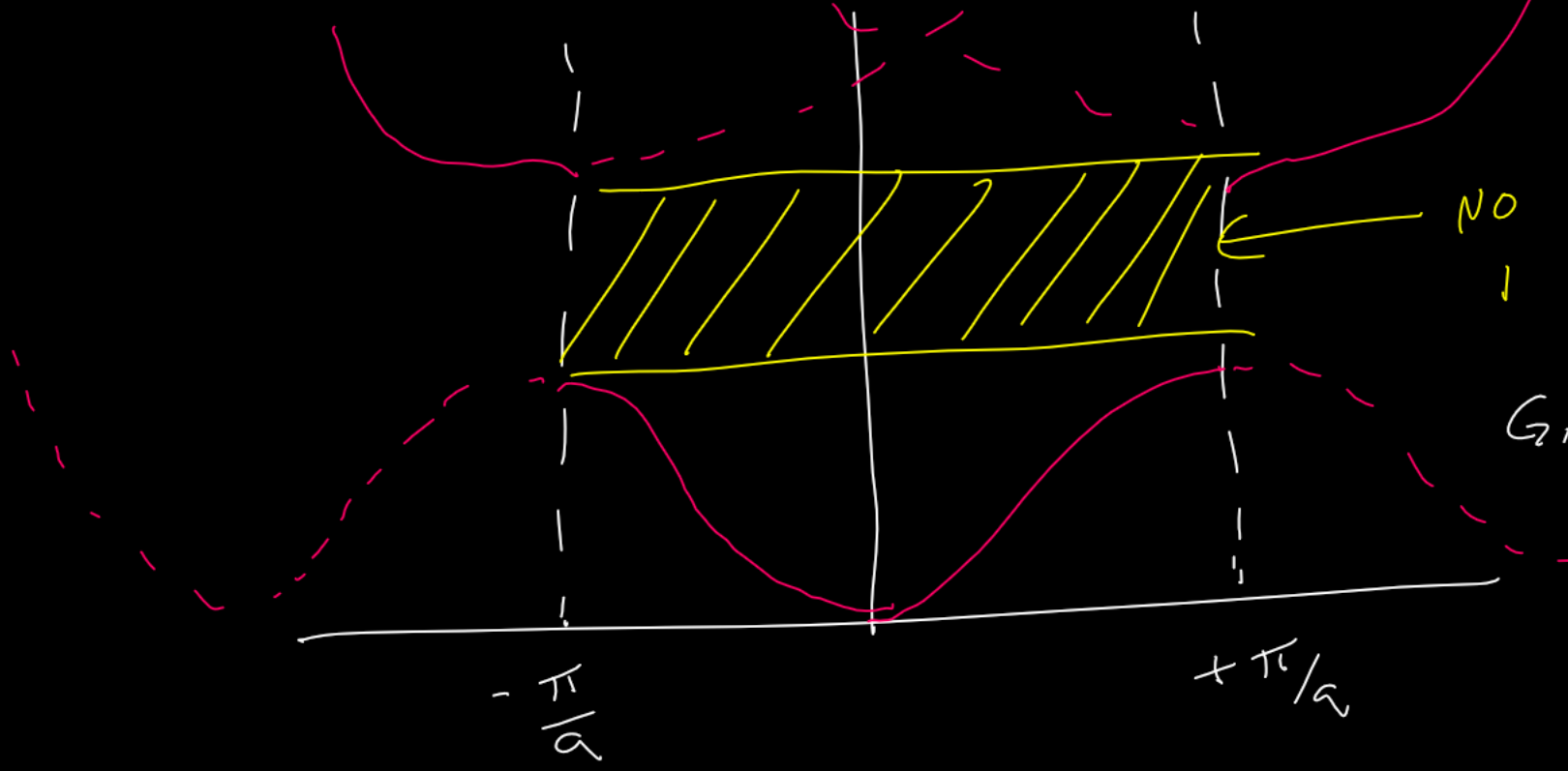
$k = \pm \frac{\pi}{a}$ $\Rightarrow$ BRAGG CONDITION (VAN LAUE)

$\Rightarrow$ X-RAYS DIFFRACTED

$\Rightarrow$ ELECTRONS DIFFRACTED

NOW PERIODIC POTENTIAL (LATTICE)

ENERGY GAP OPENS AT B.Z. BOUNDARY IN ELECTRON ENERGY SPECTRUM



NO PROPAGATING SOLNS 1 PARTICLE SCH. EQ.

GAP $\sim 2|U_K|$

$\Rightarrow$ WAVE FUNCTIONS NO LONGER $e^{\pm i\frac{\pi}{a}x}$

$\Rightarrow$ STANDING WAVES $\cos\frac{\pi}{a}x$, $\sin\frac{\pi}{a}x$

$\cos\frac{\pi}{a}x$ $\Downarrow$ LOWER

$\sin\frac{\pi}{a}x$ $\Downarrow$ HIGHER

GAP EXPLAINS PROPERTIES OF MATERIALS

1. METAL (INCOMPLETELY FILLED BAND)
2. INSULATORS (FILLED BANDS)
3. SEMICONDUCTORS

* *

BLOCH'S THEOREM

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

$$U(\vec{r}) = U(\vec{r} + \vec{R}) \quad \forall \ \vec{R} \in D.L.$$

PERIODIC POTENTIAL

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

PERIODIC

n → BAND INDEX

$\vec{k}$ → BLOCH INDEX (WAVEVECTOR)

NOTE: (1)

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

$e^{i\vec{k}\cdot\vec{R}}$ ⇑ PHASE

② $\hbar\vec{k}$ IS NO LONGER THE MOMENTUM.

$$\frac{\hbar}{i}\nabla \; \psi_{n\vec{k}}(\vec{r}) \neq \hbar\vec{k}$$

$\frac{\hbar}{i}\nabla \rightsquigarrow \hat{p}$

③ 1-D $\Rightarrow$ FLOQUET'S THM

④ $\vec{k}$ CAN BE ALWAYS RESTRICTED TO 1ST B.Z.

$$\vec{k}' = \vec{k} + \vec{K}$$

$\vec{K}$ ∈ R.L.

$$e^{i\vec{k}'\cdot\vec{R}} = e^{i\vec{k}\cdot\vec{R}}\, e^{i\vec{K}\cdot\vec{R}}$$

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

⑤ IF WE TREAT THROUGH ALL "K" SPACE $\Rightarrow$ PERIODIC IN k-SPACE

$$\psi_{n\,\vec{k}+\vec{K}}(\vec{r}) = \psi_{n,\vec{k}}(\vec{r})$$

$$\varepsilon_{n,\vec{k}+\vec{K}} = \varepsilon_{n,\vec{k}} \Longrightarrow$$

"ELECTRONIC STRUCTURE"

BAND STRUCTURE

⑥ CAN SHOW

$\varepsilon_n(\vec{k})$ ← ENERGY LEVEL (EIGENVALUE)

$$V_{n,\vec{k}} = \frac{\nabla_{\vec{k}}}{\hbar}\,\varepsilon_n(\vec{k}) \Rightarrow \frac{\partial}{\partial k}\omega(k) \Rightarrow V_g$$

$V_{n,\vec{k}}$ ⇑ AVERAGE VELOCITY

$$\frac{\omega}{k} = V_{PH}$$

IN SPITE OF INTERACTIONS ELECTRON & LATTICE

$\Longrightarrow$ ELECTRON TRAVELS WITH $V_{n,\vec{k}}$ &

DOES NOT SCATTER

PROOF OF BLOCH'S THM

DISCRETE TRANSLATION OPERATOR $\hat{T}_a$

$$\hat{T}_a \psi(x) = \psi(x+a)$$

EIGENFUNCTIONS $\phi(x)$ OF $\hat{T}_a$

$$\hat{T}_a \phi(x) = \lambda \phi(x) \qquad \lambda = \text{EIGENVALUE}$$

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

$\hat{T}_a$ IS UNITARY $\quad |\lambda| = 1$

$$\phi(x+a) = \underbrace{e^{ika}}_{\lambda}\,\phi(x)$$

$$\phi(x) = e^{ikx}\,u(x)$$

$$\hat{T}_a\,\phi(x) = e^{ik(x+a)}\,u(x+a) = e^{ika}\,\phi(x)$$

$$= e^{ik(x+a)}\,u(x)$$

$$\Rightarrow \quad u(x+a) = u(x)$$

$$[\hat{H}, \hat{T}_a] = 0 \quad \Rightarrow \quad \text{SIMULTANEOUS EIGEN FUNCTIONS}$$

$$\psi_{nk}(x) = e^{ikx} u_{nk}(x)$$

$$u_{nk}(x+a) = u_{nk}(x)$$