LECTURE # 17

Note Title 10/29/2008

CuO_2

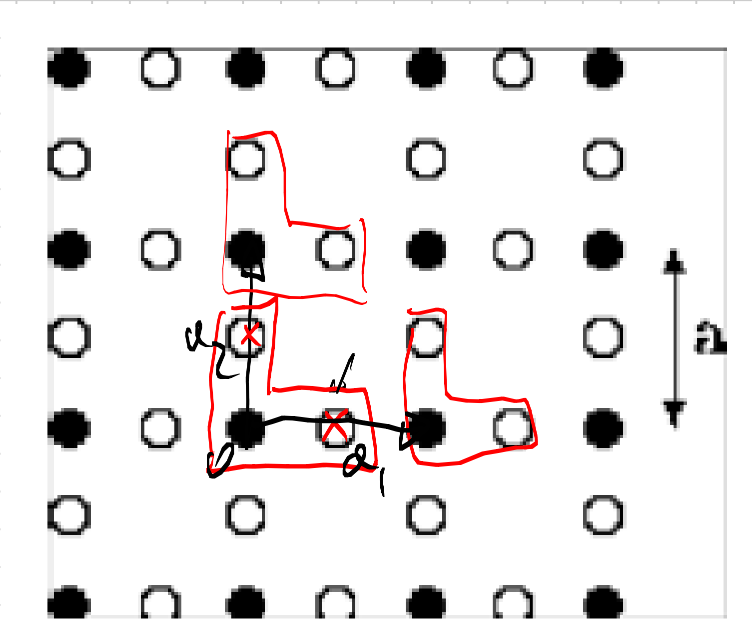


Figure 1.6: CuO_2 lattice

$$\vec{a}_1 = a(1\ 0)$$

$$\vec{a}_2 = a(0\ 1)$$

$$\vec{R}_i = m\vec{a}_1 + m\vec{a}_2$$

BASIS

$$\vec{d}_{Cu} = 0$$

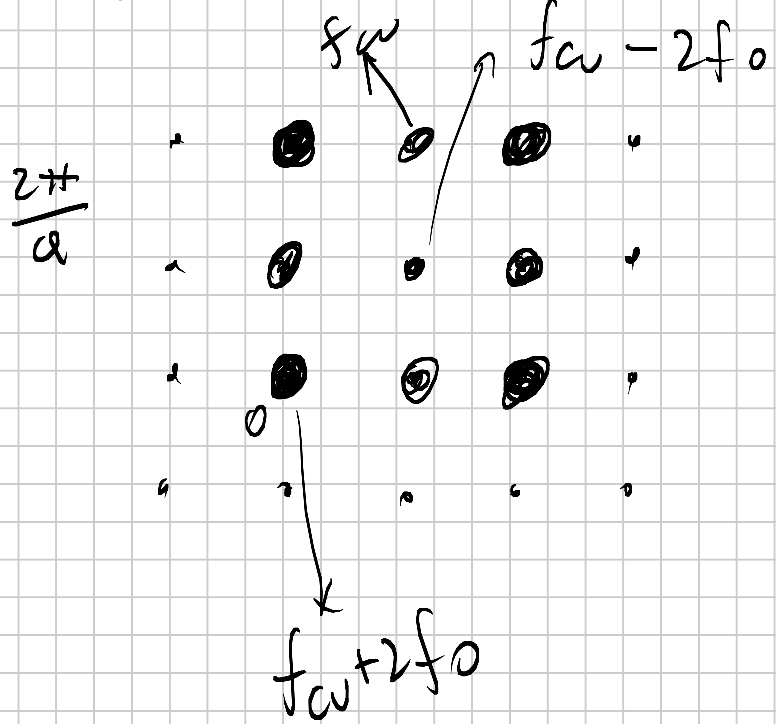
$$\vec{d}_{O_1} = a\left(\tfrac{1}{2}\ 0\right)$$

$$\vec{d}_{O_2} = a\left(0\ \tfrac{1}{2}\right)$$

Cu f_{Cu}

O f_O

RECIPROCAL LATTICE



$$\vec{b}_1 = \frac{2\pi}{a}(1,0)$$

$$\vec{b}_2 = \frac{2\pi}{a}(0,1)$$

$$\vec{K} = m_1\vec{b}_1 + m_2\vec{b}_2 =$$

$$= \frac{2\pi}{a}\left(m_1\hat{x} + m_2\hat{y}\right)$$

STRUCTURE FACTOR

$$S(\vec{K}) = f_{Cu}\, e^{i\vec{K}\cdot\vec{d}_{Cu}} + f_O\, e^{i\vec{K}\cdot\vec{d}_{O_1}} + f_O\, e^{i\vec{K}\cdot\vec{d}_{O_2}} =$$

$$\frac{2\pi}{a}\left(m_1\hat{x} + m_2\hat{y}\right)\cdot\frac{a}{2}\hat{x} = \pi m_1$$

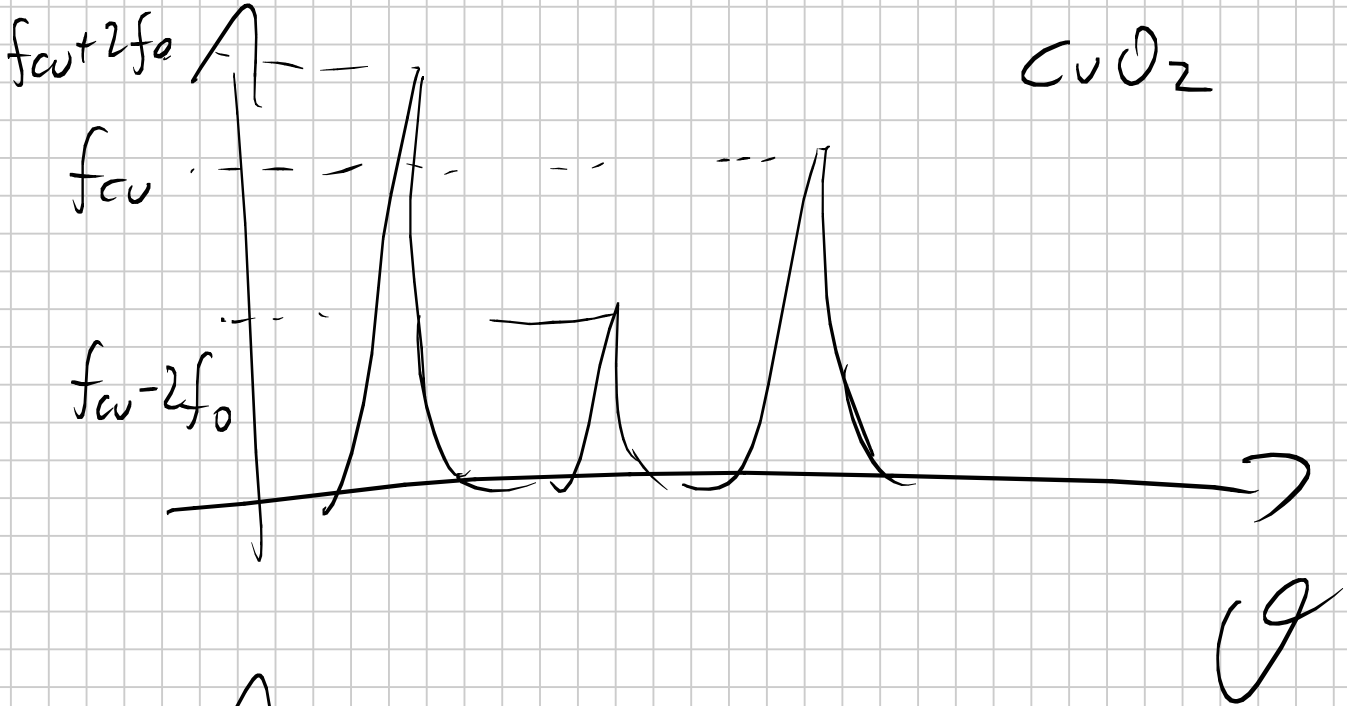
$$S(\vec{K}) = f_{cu} + f_0\left(e^{im_1\pi} + e^{im_2\pi}\right)$$

m_1 & m_2 EVEN $\quad f_{cu} + 2f_0$

m_1 & m_2 ODD $\quad f_{cu} - 2f_0$

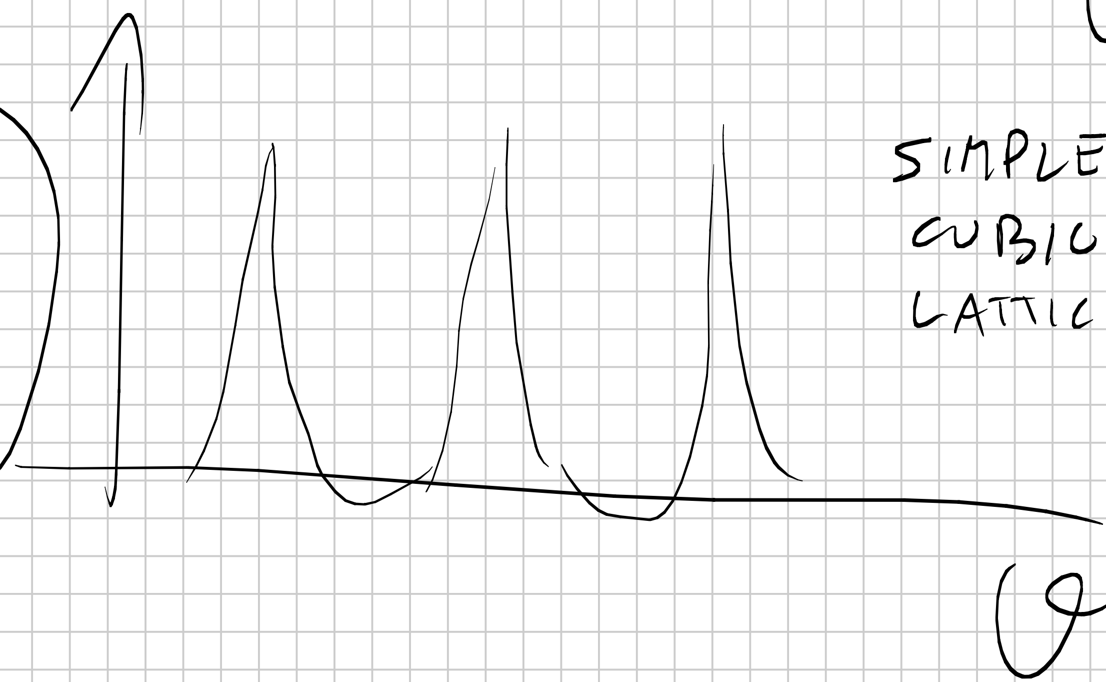
m_1, m_2 ONE EVEN ONE ODD $\quad f_{cu}$

X-RAY PEAKS



CuO_2

$$e^{im\pi} = \cos m\pi + i \sin m\pi$$



SIMPLE CUBIC LATTICE

ELECTRONIC STATES IN A PERIODIC POTENTIAL $V_{ION}(\vec{r})$

① BLOCH'S THEOREM

$$\psi_{m\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{m\vec{k}}(\vec{r})$$ WHERE $u(\vec{r})$ PERIODIC

② $\vec{k}$ CRYSTAL MOMENTUM

③ $\psi_{\vec{k}}$, $\psi_{\vec{k}+\vec{K}}$ <u>SAME STATE</u>

$\underline{K}$ RECIPROCAL LATTICE VECTOR

④ $E(\vec{k}) = E(\vec{k}+\vec{\underline{K}}) \quad \forall \; \underline{K}$

ENERGY PERIODIC IN K SPACE

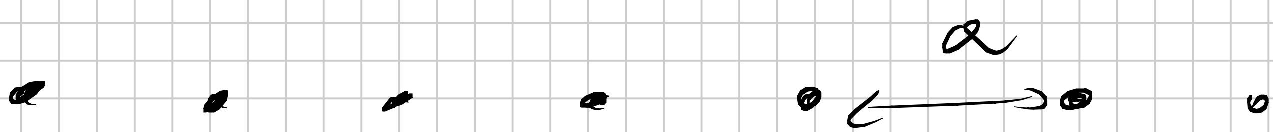
PERIODICITY OF THE RECIPROCAL LATTICE

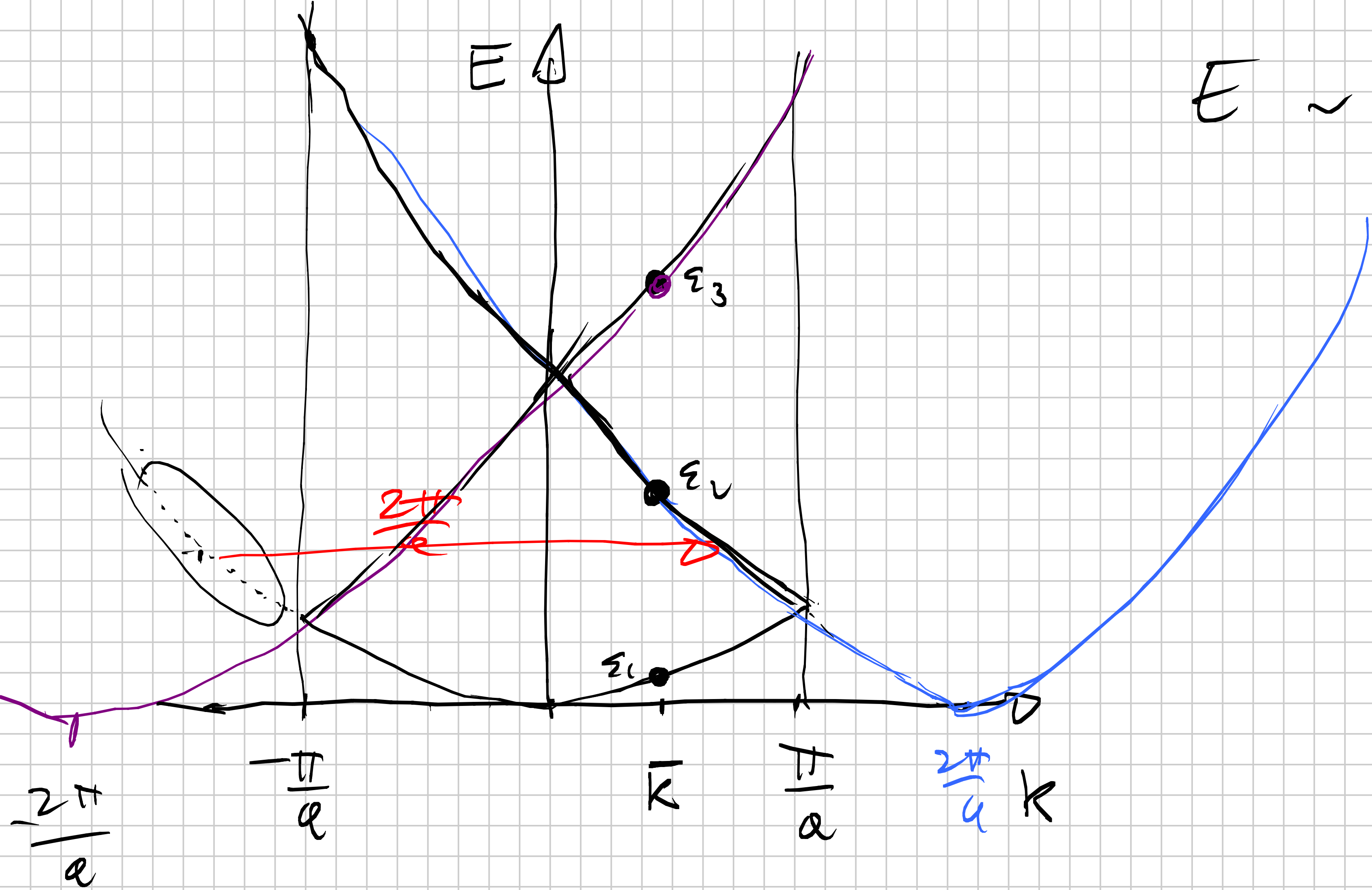
⑤ LOOK AT ELECTRONIC STATES ON THE 1° BRILLOUIN ZONE

NEARLY FREE ELECTRONS

$V_{ION} \sim 0$

1D SYSTEM



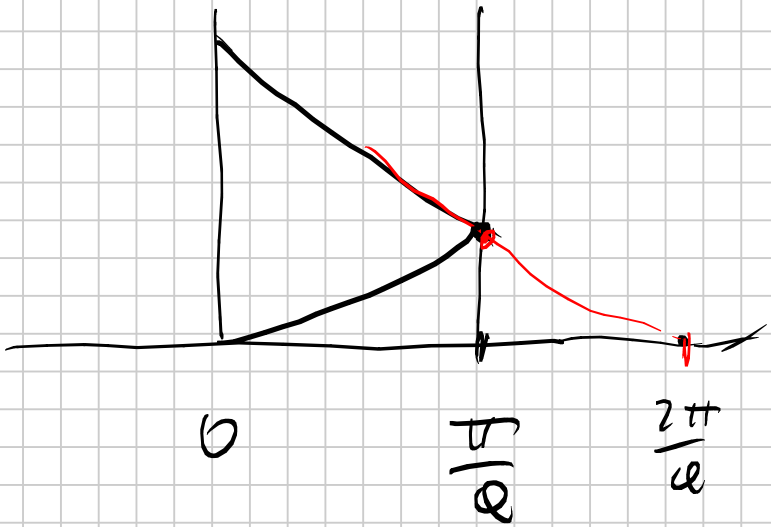


$$E \sim \frac{\hbar^2 k^2}{2m}$$

FOR CRYSTAL MOMENTUM $\bar{k}$

$$\varepsilon_1 = \frac{\hbar^2 \bar{k}^2}{2m}, \qquad \varepsilon_2 = \frac{\hbar^2 \left(\bar{k} - \frac{2\pi}{a}\right)^2}{2m}$$

$$\varepsilon_3 = \frac{\hbar^2 \left(\bar{k} + \frac{2\pi}{a}\right)^2}{2m}$$



LOOK AT POINT

$k = \frac{\pi}{a}$

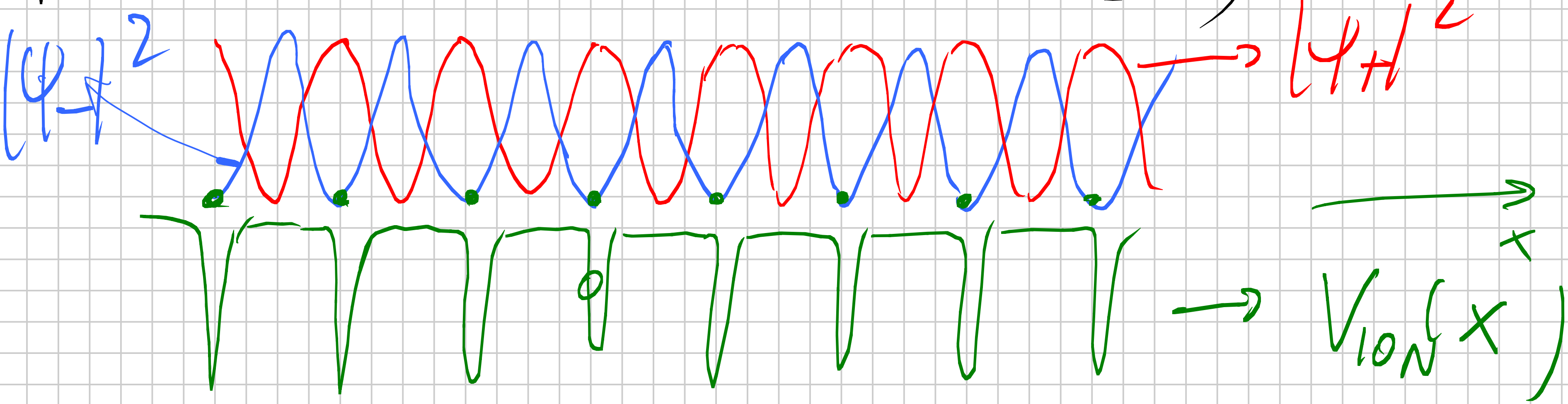
e^{ikx} FOR $k = \frac{\pi}{a}$ $= e^{i\frac{\pi}{a}x}$

$$\psi_1 = e^{i\frac{\pi}{a}x}$$

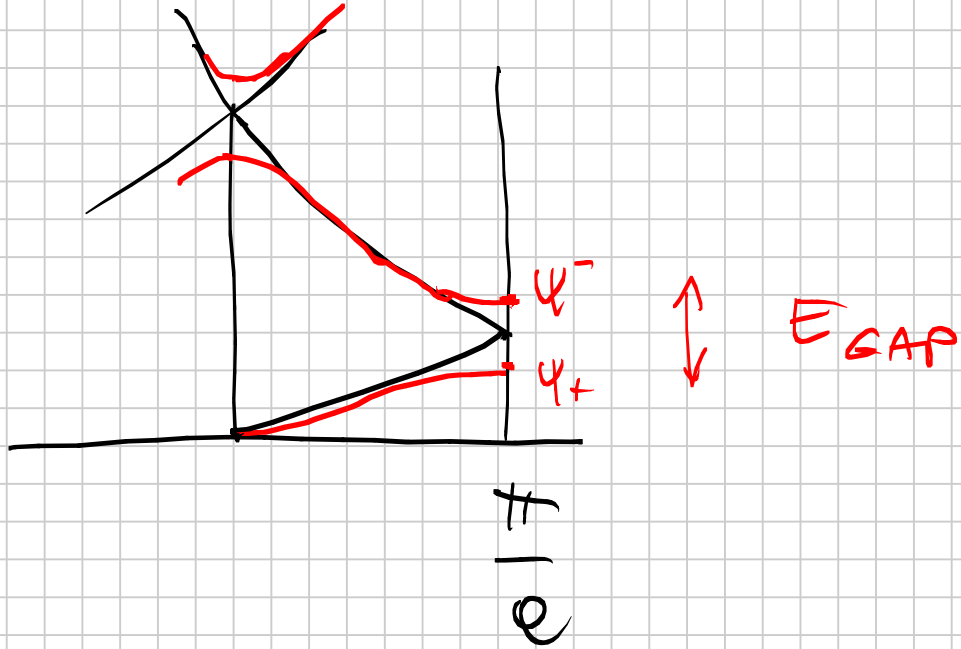
$$\psi_2 = e^{i\left(k - \frac{2\pi}{a}\right)x} = e^{-i\frac{\pi}{a}x}$$

$$\psi_+ = e^{i\frac{\pi}{a}x} + e^{-i\frac{\pi}{a}x} \sim 2\cos\left(\frac{\pi}{a}x\right)$$

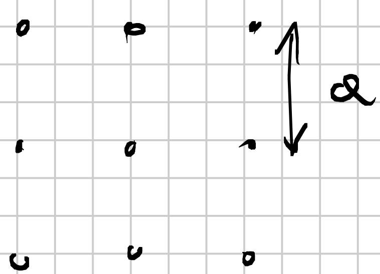
$$\psi_- = e^{i\frac{\pi}{a}x} - e^{-i\frac{\pi}{a}x} \sim 2i\sin\left(\frac{\pi}{a}x\right)$$

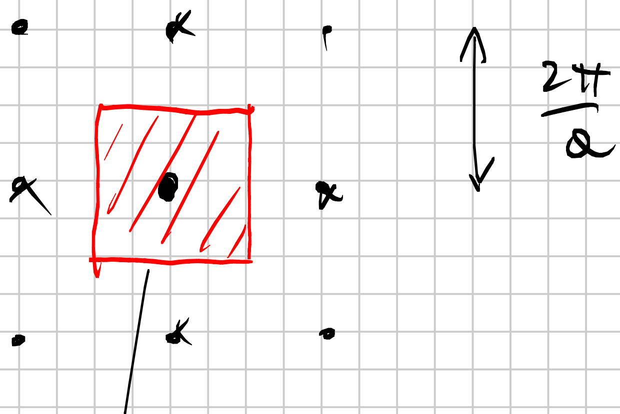


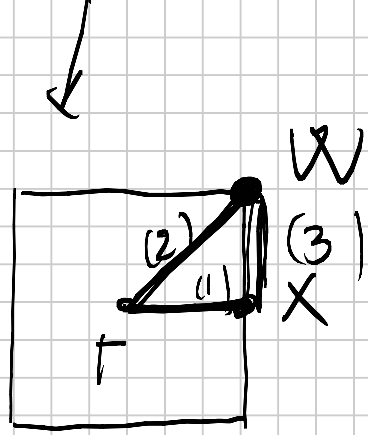
ψ_+ HAS LOWER ENERGY BECAUSE INTERACTS MORE WITH $V_{ION}(x)$ THAN ψ_-



V_{ION} SMALL



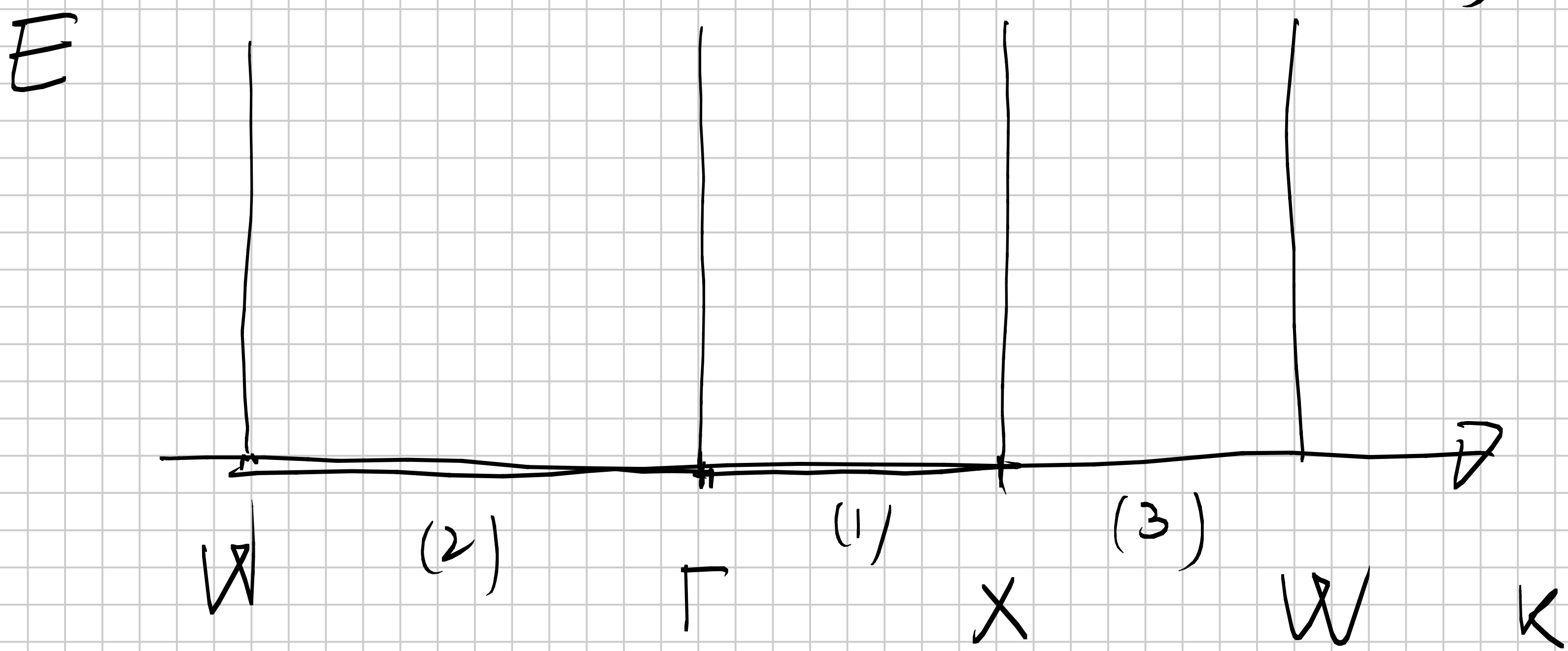




$\Gamma = (0, 0)$

$X = \left(\frac{\pi}{a}, 0\right)$

$W = \left(\frac{\pi}{a}, \frac{\pi}{a}\right)$



$$E = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2\right)$$