Lecture 9

Electrons in Crystal

Nearly free electron model

Tight binding model

Bloch's Theorem

- See Note

Form 1 of Bloch Theorem [BL translation eigenstate, Crystal momentum eigenstate]

$\psi_{n\vec{k}}(\vec{x}+\vec{R}) = \exp(i\vec{k}\cdot\vec{R})\psi_{n\vec{k}}(\vec{x})$ for any $\vec{R} \in$BL.

Form 2 of Bloch Theorem [Bragg diffraction of plane wave; Nearly free electron]

$\psi_{n\vec{k}}(\vec{x}) = \sum_{\vec{G}} C_n(\vec{G}) \exp\left[i(\vec{k}+\vec{G})\cdot\vec{x}\right]$

Form 3 of Bloch Theorem [Modulated plane wave; Nearly free electron]

$\psi_{n\vec{k}}(\vec{x}) = \exp(i\vec{k}\cdot\vec{x})u_{n\vec{k}}(\vec{x})$ where $u_{n\vec{k}}(\vec{x}+\vec{R}) = u_{n\vec{k}}(\vec{x})$ for any $\vec{R} \in$BL.

Form 4 of Bloch Theorem [Modulated local wave function; phonon or tight-binding electron]

$\psi_{n\vec{k}}(\vec{x}) = \sum_{\vec{R}} \exp(i\vec{k}\cdot\vec{R})\phi_n(\vec{x}-\vec{R})$

Dynamical Origin of Bloch's Theorem

- Hamiltonian $H = T + V$
- In the plane wave basis,

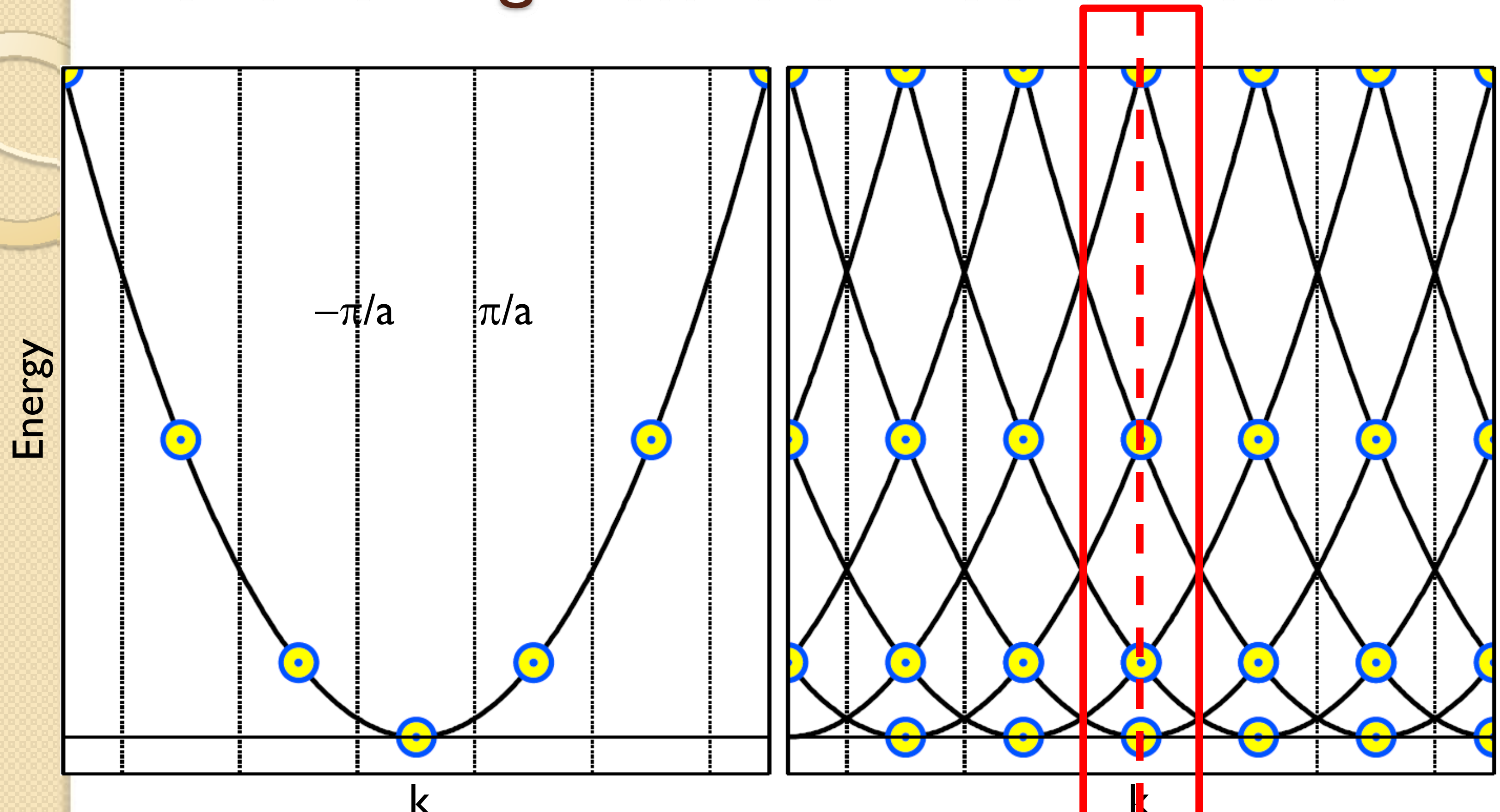
$$H = \Sigma_{k,G} |k\rangle\langle k|H|k+G\rangle\langle k+G|$$

As T is already diagonal, it only needs to be seen that
$V = \Sigma_{k,k'} |k\rangle\langle k|V|k'\rangle\langle k'| = \Sigma_{k,K} |k\rangle\langle k|V|k+G\rangle\langle k+G|$.

The last step is the most important (G = R.L. vector), following from the translation symmetry of the crystal.

- Thus, an eigenstate = $\Sigma_{k,G} C(G)|k+G\rangle$

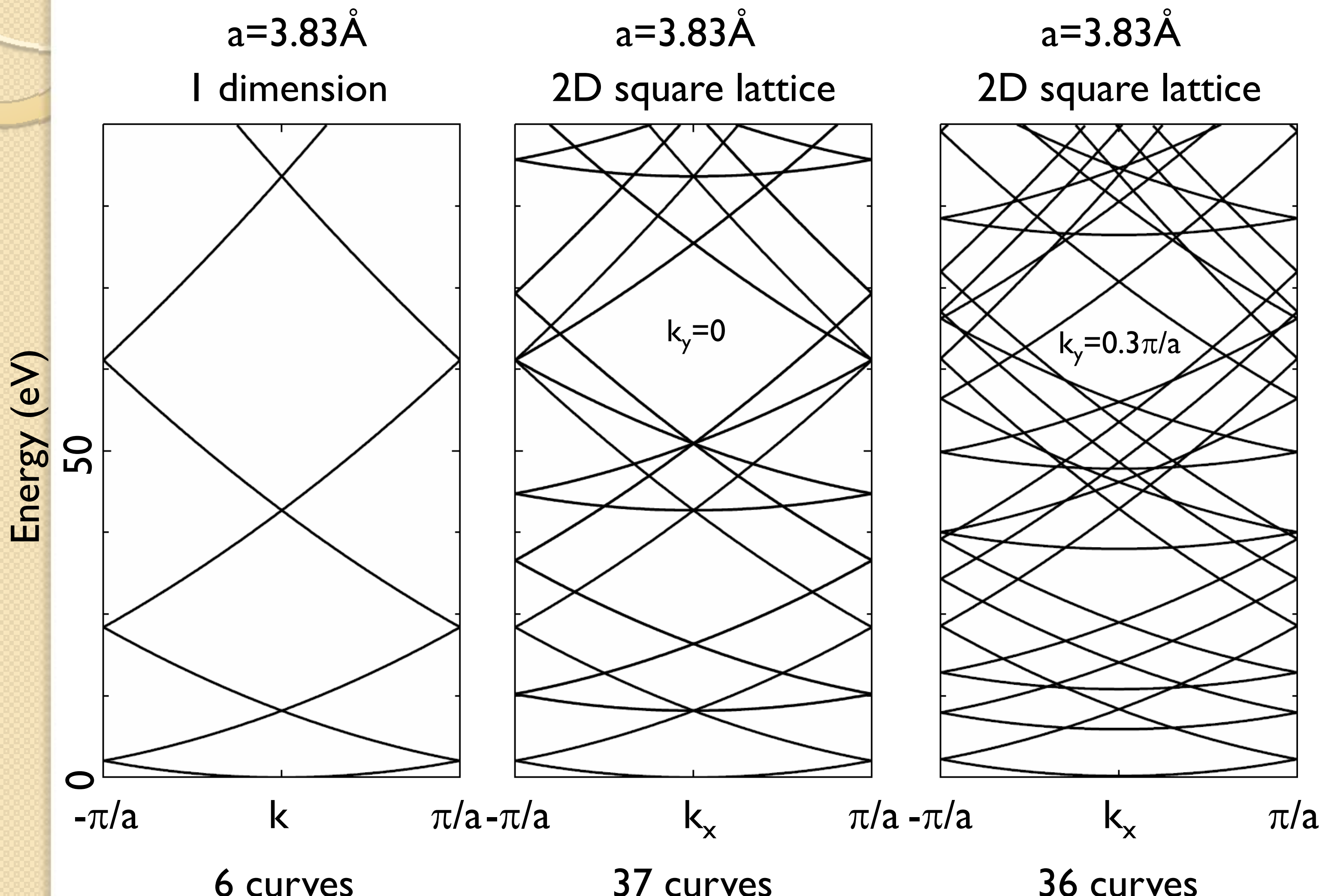
Zone Folding Picture of Bloch's Theorem



Procedure to solve for <u>any</u> crystal potential (not only for weak potential)

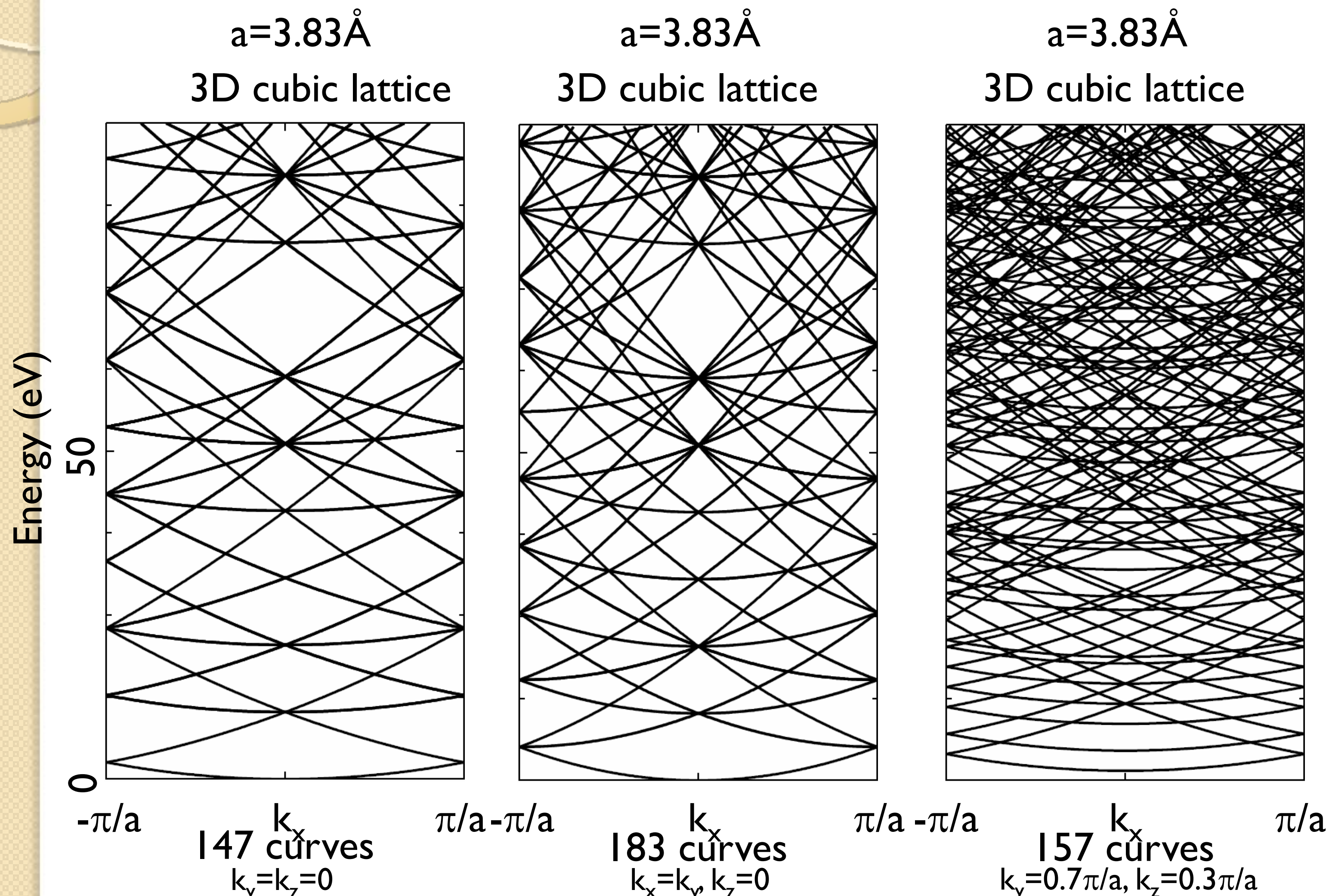
1. Start from plane wave
2. Fold the free electron band to the first Brillouin zone
3. Solve the block matrix of H for states along a vertical line

Zone-Folding and dimensionality



Zone-Folding and dimensionality

Curves ~ A^D, for a given energy range (0 – 100 eV here; with A = 5-6)



Equation of Motion

∞ x ∞ matrix !

$$
\begin{bmatrix}
 & \ddots & \vdots & \vdots & \vdots & \iddots \\
V(1) & \lambda_{k-G}-E & V(1)^* & V(2)^* & V(3)^* & \cdots \\
V(2) & V(1) & \lambda_{k}-E & V(1)^* & V(2)^* & \cdots \\
\cdots & V(2) & V(1) & \lambda_{k+G}-E & V(1)^* & \cdots \\
\iddots & \vdots & \vdots & \vdots & \ddots &
\end{bmatrix}
\begin{bmatrix}
\vdots \\
C(k-G) \\
C(k) \\
C(k+G) \\
\vdots
\end{bmatrix}
= 0
$$

Toy Problem (Kronig-Penney)

$$V(x) = Aa\sum_{n=1}^{N}\delta(x-na)$$

$$V(G) = \frac{1}{L}\int_0^L dx\, V(x)\exp(-iGx) = \frac{1}{L}Aa\sum_{n=1}^{N}\exp(-iGna)\,,\quad G = integer\times\frac{2\pi}{a}$$

$$V(G) = \frac{1}{L}AaN = \frac{AL}{L} = A$$

$$N\to\infty$$

$$(\lambda_k - E)C(k) + A\sum_{n=-\infty}^{\infty}C\left(k-\frac{2\pi n}{a}\right) = 0$$

$$f(k) \equiv \sum_{n=-\infty}^{\infty}C\left(k-\frac{2\pi n}{a}\right)$$

$$C(k) = -\frac{Af(k)}{\lambda_k - E}$$

$$f\left(k-\frac{2\pi m}{a}\right) = f(k),\qquad m = any\ integer$$

$$f(k) = \sum_{n=-\infty}^{\infty}C\left(k-\frac{2\pi n}{a}\right) = \sum_{n=-\infty}^{\infty}-\frac{Af(k)}{\lambda_{k-2\pi n/a}-E}$$

$$1 = -\sum_{n=-\infty}^{\infty}\frac{A}{\lambda_{k-2\pi n/a}-E}$$

$$E = \frac{\hbar^2K^2}{2m}$$

$$A = \frac{\hbar^2P^2}{2m}$$

$$\cot(x) = \sum_{n=-\infty}^{\infty}\frac{1}{n\pi + x}$$

a bit of math

$$\frac{\hbar^2}{2mA} = -\sum_{n=1}^{N}\frac{1}{\left(k-\frac{2\pi n}{a}\right)^2 - K^2} = \frac{a^2\sin(Ka)}{4Ka(\cos(ka)-\cos(Ka))}$$

$$\frac{P\sin(Ka)}{Ka} + \cos(Ka) = \cos(ka)$$

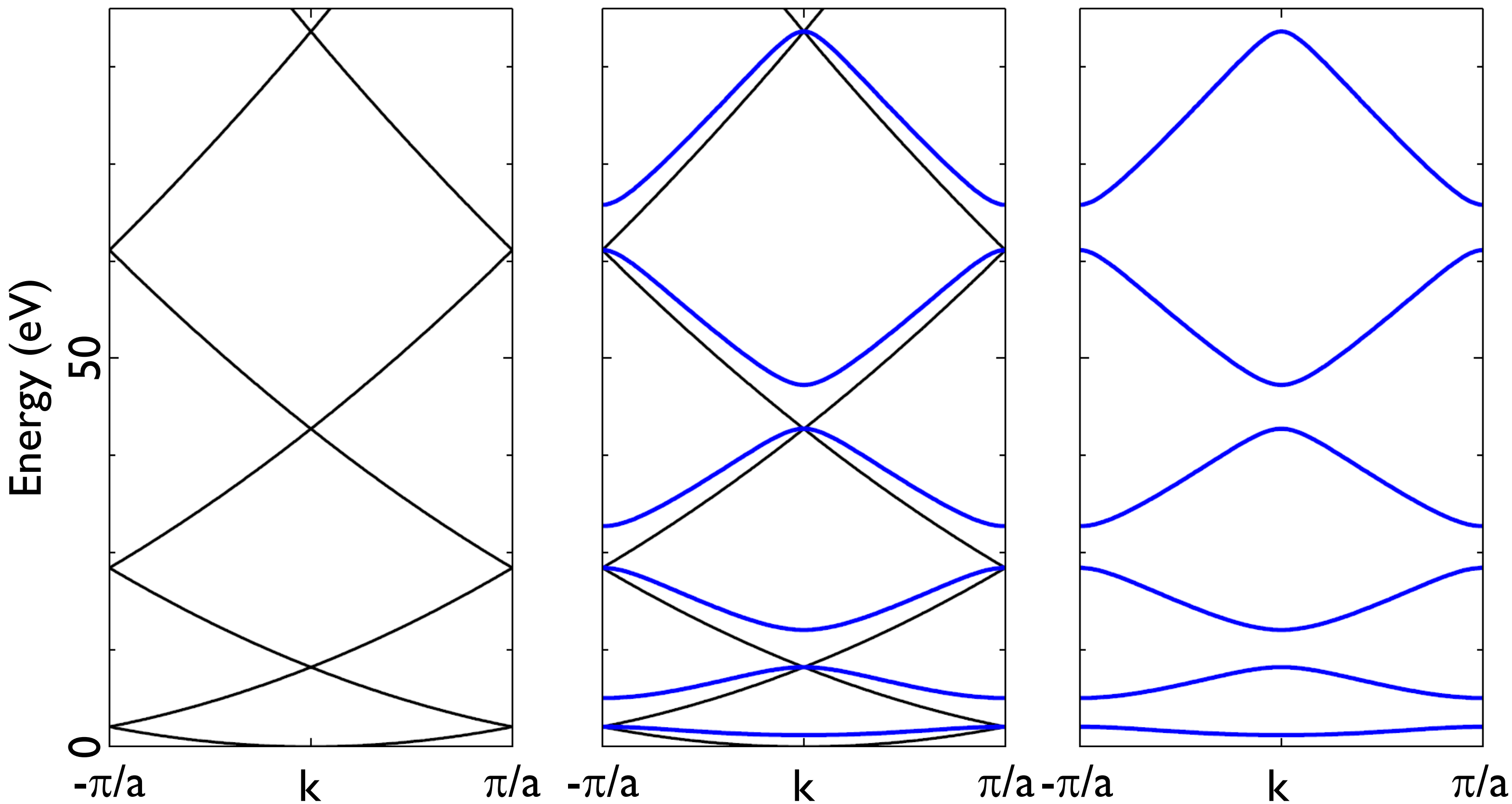
$$P = \frac{mAa^2}{2\hbar^2}$$

Toy Problem (Kronig-Penney)

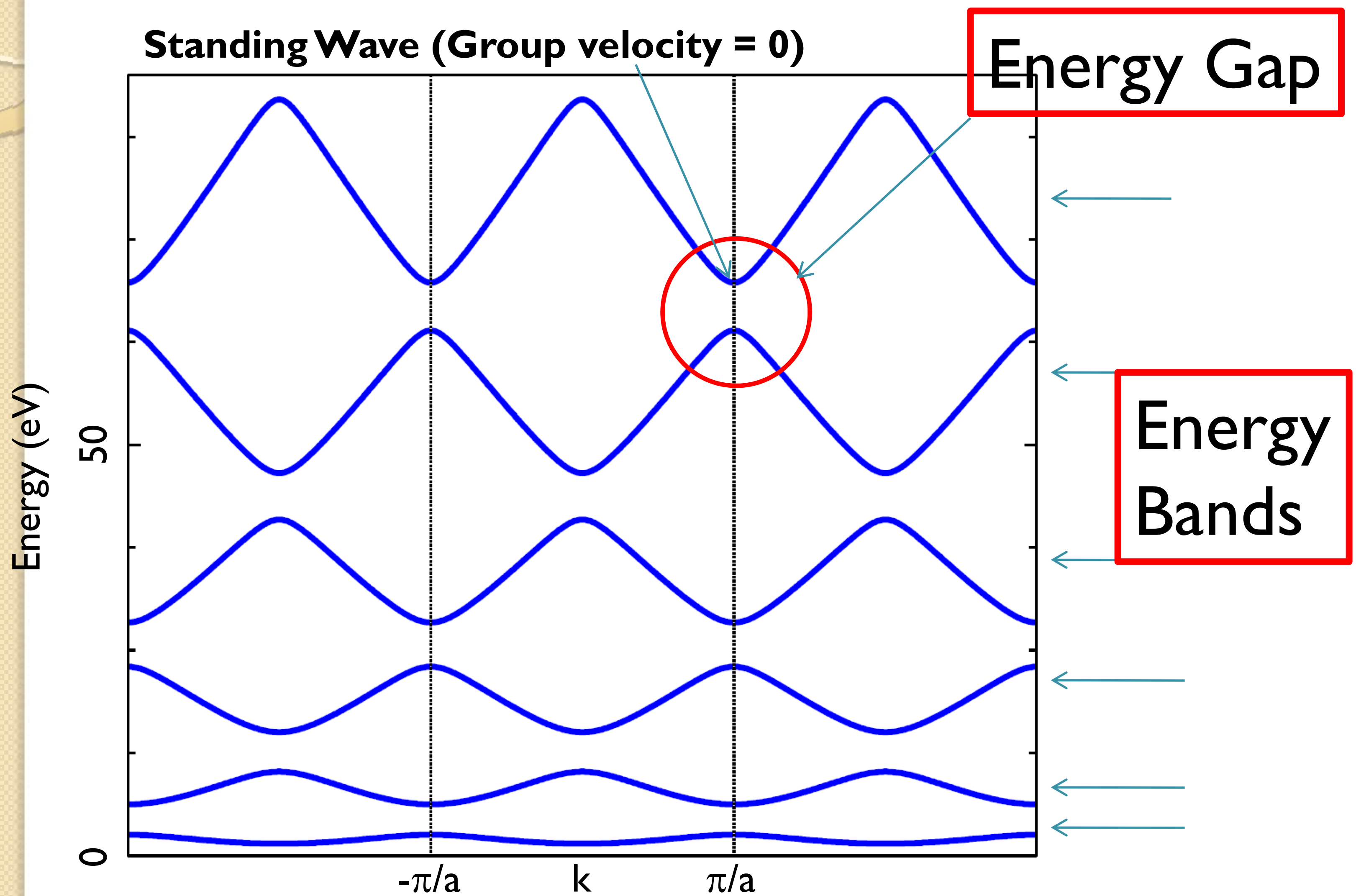
$$\frac{P\sin(Ka)}{Ka} + \cos(Ka) = \cos(ka)$$

$$P = \frac{mAa^2}{2\hbar^2}$$

a=3.83Å
P = 6



Toy Problem (Kronig-Penney)



Good News! 2x2 Problem!

Consider a Hamiltonian for two states |0>, |1> interacting with each other

$$\begin{bmatrix} 0 & V \\ V^* & 0 \end{bmatrix}$$

$V=|V|\exp(i\delta)$

Eigen-values = $\pm |V|$

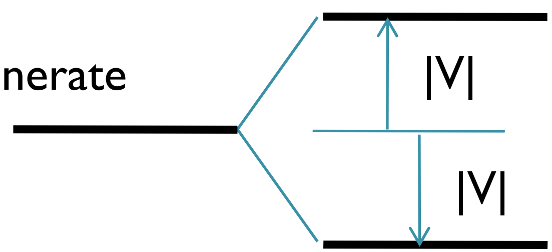
Equal parts of |0> and |1>

Eigen-state = |0> - exp($-i\delta$) |1>, for Eigen-value = -|V| (ground state)
|0> + exp ($i\delta$) |1>, for Eigen-value = |V| (excited state)

Up to a normalization factor (1/sqrt(2))

"Anti-Bonding"

degenerate

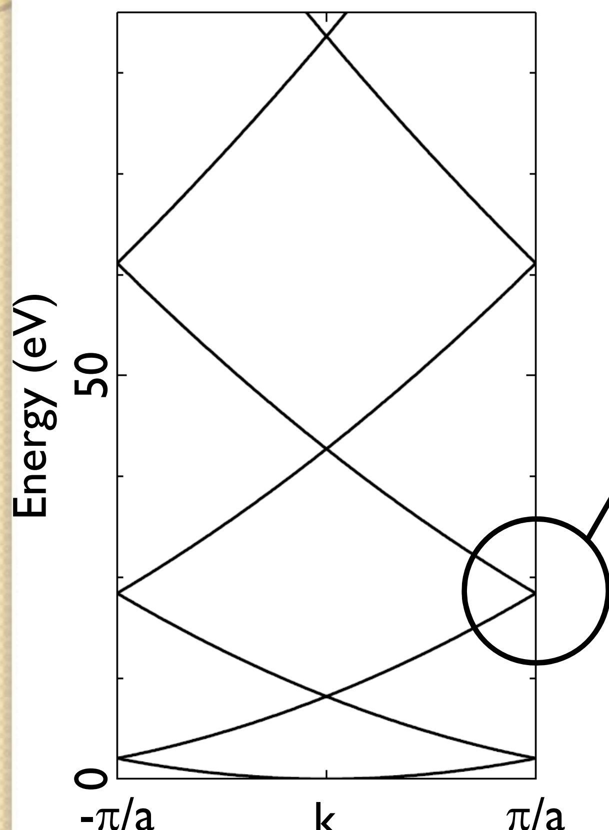


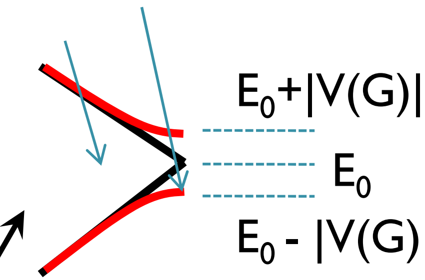
"Bonding"

V real negative ($\delta=\pi$)	V real positive ($\delta=0$)
|0> -|1>	|0> +|1>
|0> +|1>	|0> -|1>

In the limit of weak potential (2x2 approx)

At $k=\pi/a$, wave function is equal mix of k and k+G
→ Standing Wave (group velocity = 0)
→ $dE / dk = 0$





General condition that energies are the same

$$|\mathbf{k}| = |\mathbf{k}-\mathbf{G}|$$

Perpendicular bi-sector planes that we used in defining the BZ (Wigner Seitz Cell)!