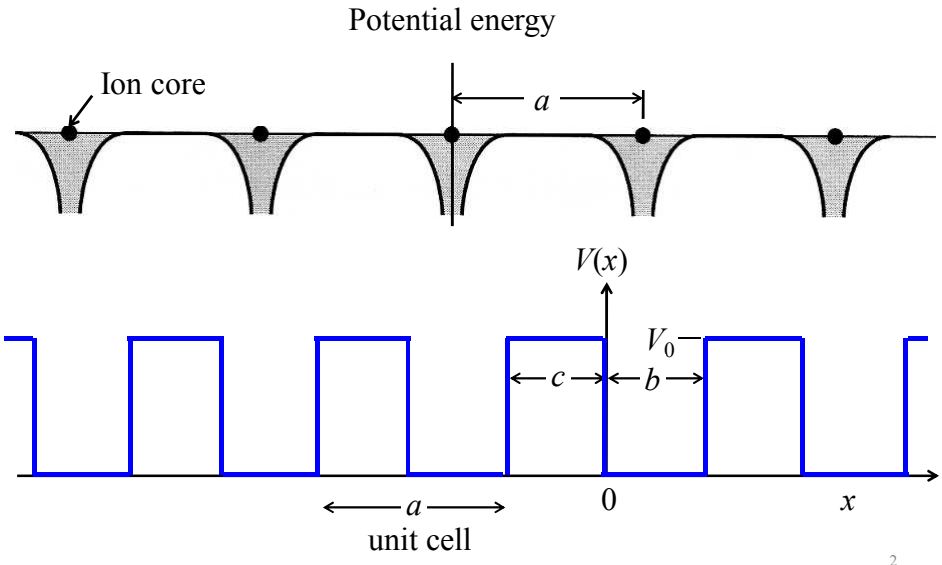
KRONIG-PENNY MODEL

Periodic Potential



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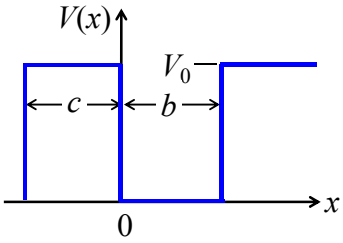
Dispersion Relation



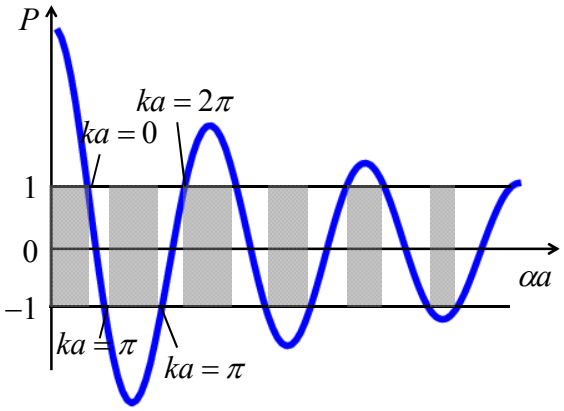
$$\left[1+\frac{V_0^2}{4\varepsilon(\varepsilon-V_0)}\sin^2\beta c\right]^{1/2}\cos(\alpha b-\delta)=\cos ka, \qquad (\varepsilon>V_0)$$

$$\left[1+\frac{V_0^2}{4\varepsilon(V_0-\varepsilon)}\sinh^2\gamma c\right]^{1/2}\cos(\alpha b-\delta')=\cos ka, \qquad (0<\varepsilon<V_0)$$

where $\alpha^2=\frac{2m\varepsilon}{\hbar^2}$ $\beta^2=\frac{2m(\varepsilon-V_0)}{\hbar^2}$ $\beta=i\gamma$

3

Energy Bands



Forbidden energy range.

- In an infinite lattice, the states within any allowed band would form a continuum.
- For a lattice of *N* atoms, there are *N* discrete states, however, there are 2*N* states for spin degeneracy.
- The energy gaps decrease as electron energy increases → free electron behavior at high energies.

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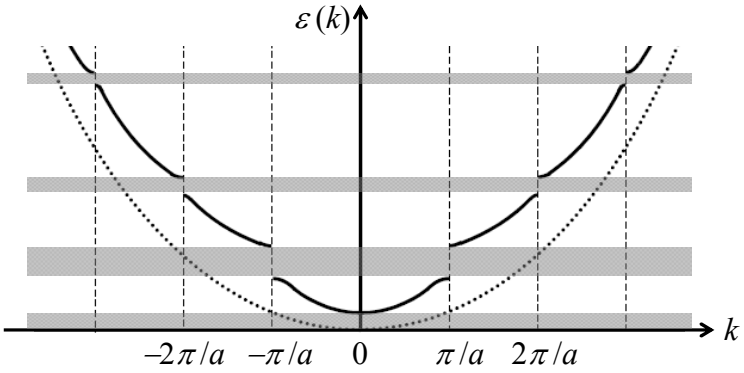
Dispersion Relation



- Energies close to zero are forbidden.
- At $k = n\pi/a$, there are two possible values of energies.
- Bragg reflection at $k = \pm n\pi/a$

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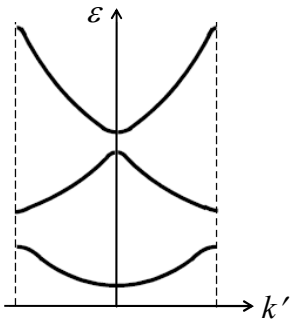
Reduced Zone Representation

- Energy band diagram is plotted in the first Brillouin zone.



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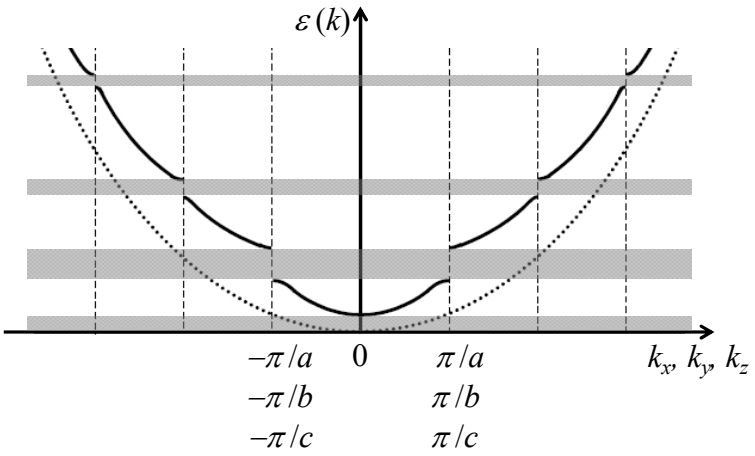
Dispersion Relation: 3D



$a = b = c$

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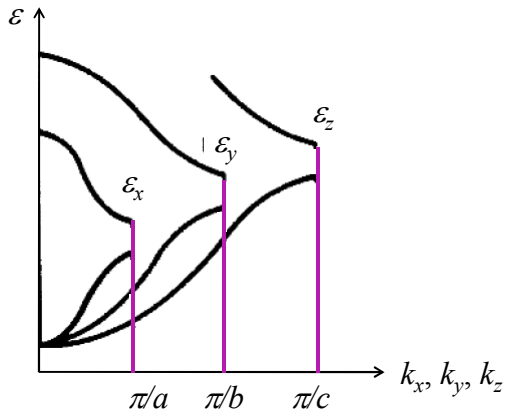
Dispersion Relation: 3-D

- k-values at the zone boundaries along different crystal orientations may be different → overlap of energy states at zone boundaries.



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TIGHT-BINDING MODEL

Concept

- Start with the energy levels of atoms and bring them closer and closer together to form a crystal.
- *Nearly free electron model* starts from the opposite end.
- First, we will solve the problem of two atoms being brought together, and then that of the crystal.

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Orthogonality

- If two states are orthogonal:

$$\int_{-\infty}^{\infty} \phi_m^*(x)\,\phi_n(x)\,dx = \delta_{mn}$$

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Single Well / Atom

- Hamiltonian of a single quantum well:

$$\hat{H} = \hat{T} + \hat{V}$$

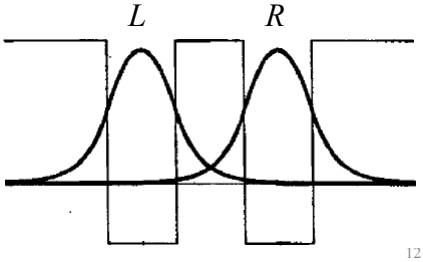
$\hat{T}$: Kinetic energy operator

$\hat{V}$: Potential energy operator

- Consider two isolated wells or atoms.

$$\left(\hat{T} + \hat{V}_L\right)\phi_L = \varepsilon\phi_L$$

$$\left(\hat{T} + \hat{V}_R\right)\phi_R = \varepsilon\phi_R$$



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Two Wells: Diatomic Molecule

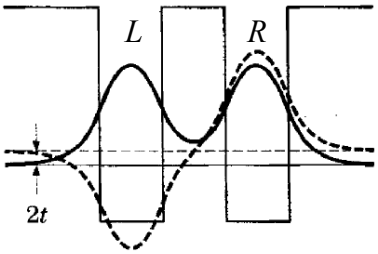
- Hamiltonian: $\hat{H} = \hat{T} + \hat{V}_L + \hat{V}_R$

  $\hat{T}$: Kinetic energy operator

  $\hat{V}_L$: Potential energy operator for left well

  $\hat{V}_R$: Potential energy operator for right well

- Wavefunction: $\psi = a_L\phi_L + a_R\phi_R$



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Schrodinger's Equation

- New wavefunction: $\psi = \sum_n a_n\phi_n$

$$\hat{H}\sum_n a_n\phi_n = E\sum_n a_n\phi_n$$

- Multiply both sides by ϕ_m* and integrate

$$\sum_n H_{mn}a_n = E\sum_n S_{mn}a_n$$

$$H_{mn} = \int \phi_m^* \hat{H}\phi_n, \quad S_{mn} = \int \phi_m^*\phi_n$$

- Matrix equation: Ha = *E*Sa

- Matrices: $\mathrm{H} = \begin{vmatrix} H_{LL} & H_{LR} \\ H_{RL} & H_{RR} \end{vmatrix}$ $\mathrm{S} = \begin{vmatrix} S_{LL} & S_{LR} \\ S_{RL} & S_{RR} \end{vmatrix}$

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Matrix Elements

- Diagonal elements:

$$H_{LL} = \int \phi_L^* \left(\hat{T} + \hat{V}_L + \hat{V}_R \right) \phi_L dx = \varepsilon + \int \phi_L^* \hat{V}_R \phi_L dx = \varepsilon - c = H_{RR}$$

- Off-diagonal elements:

$$H_{RL} = \int \phi_R^* \left(\hat{T} + \hat{V}_L + \hat{V}_R \right) \phi_L dx = \varepsilon \int \phi_R^* \phi_L dx + \int \phi_R^* \hat{V}_R \phi_L dx = \varepsilon s - t = H_{LR}$$

$$\mathrm{H} = \begin{vmatrix} \varepsilon - c & \varepsilon s - t \\ \varepsilon s - t & \varepsilon - c \end{vmatrix}$$

c : crystal field
t : transfer, tunneling, overlap integral
s: non-orthogonality

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Matrix Elements

- Diagonal elements:

$$S_{LL} = \int \phi_L^* \phi_L dx = 1$$

- Off-diagonal elements:

$$S_{RL} = \int \phi_R^* \phi_L dx = s$$

$$\mathrm{S} = \begin{vmatrix} 1 & s \\ s & 1 \end{vmatrix}$$

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Energy Levels

- Determinants:

$$\det\left|E\mathrm{S}-\mathrm{H}\right|=0$$

$$\det\begin{vmatrix} E-\varepsilon+c & Es-\varepsilon s+t \\ Es-\varepsilon s+t & E-\varepsilon+c \end{vmatrix}=0$$

- Roots:

$$E_{-}=\varepsilon-\frac{c}{1+s}-\frac{t}{1+s}$$

$$E_{+}=\varepsilon-\frac{c}{1-s}+\frac{t}{1-s}$$

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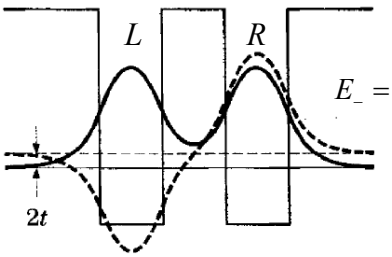
Two Wells: Diatomic Molecule



$$E_{-}=\varepsilon-\frac{c}{1+s}-\frac{t}{1+s},\quad E_{+}=\varepsilon-\frac{c}{1-s}+\frac{t}{1-s}$$

- Energy gap: $E_{+}-E_{-}=\dfrac{c}{1+s}-\dfrac{c}{1-s}+\dfrac{t}{1-s}+\dfrac{t}{1+s}\approx 2t$
- Oscillation frequency: $\omega=\dfrac{\left|E_{+}-E_{-}\right|}{\hbar}=\dfrac{2\left|t\right|}{\hbar}$

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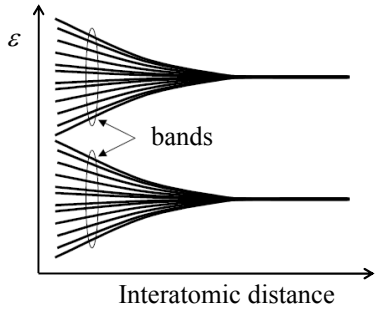
Tight-Binding Solid

- Bringing a pair of wells together caused the energy level to split into two levels separated by $2t$.
- The splitting increases as the separation decreases and the overlap t grows
- Bringing N wells together causes their common energy level to split into N values and merge into a continuous band as $N \rightarrow \infty$.



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Class Test – 2

Day: 12 December 2018

Syllabus: Lectures 9 – 12

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