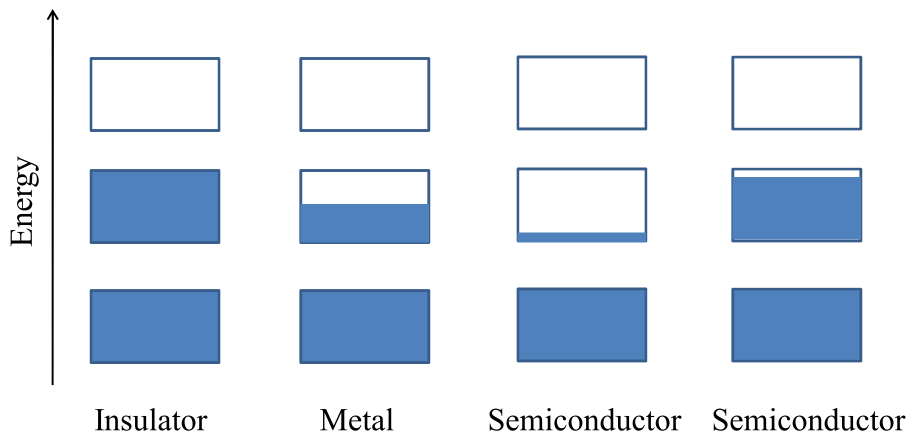
ELECTRONIC BAND STRUCTURE

Energy Bands



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Bloch Theorem

- **Bloch wave:** A type of wavefunction for a particle in a periodically repeating environment → consider an electron in a crystal.
- A wavefunction ψ is a Bloch wave if it has the form:

$$\psi\left(\vec{k},\vec{r}\right)=e^{i\vec{k}\cdot\vec{r}}\,u\left(\vec{k},\vec{r}\right)$$

$u\left(\vec{k},\vec{r}\right)$: Periodic function with the same periodicity as the crystal

$$u\left(\vec{k},\vec{r}+\vec{R}\right)=u\left(\vec{k},\vec{r}\right)$$

A plane wave modulated by a function that has periodicity of the potential.

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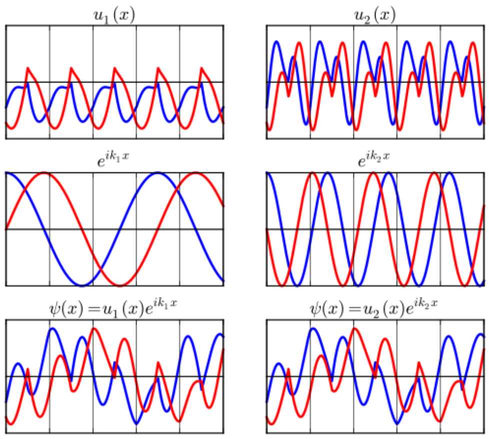
Bloch Theorem



A Bloch wave (bottom) can be broken up into the product of a periodic function (top) and a plane-wave (center). Blue is real part, red is imaginary part. The left side and right side represent the same Bloch wave broken up in two different ways, involving the wave vector k_1 (left) or k_2 (right). The difference $(k_1{-}k_2)$ is a reciprocal lattice vector.

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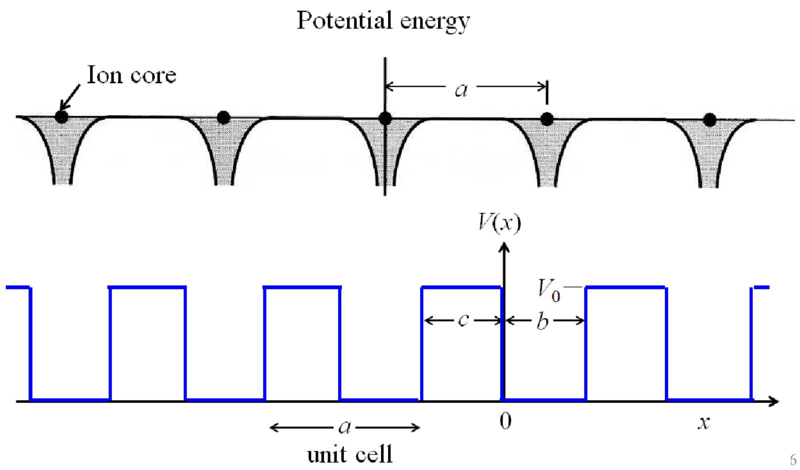
Electronic Band Structure

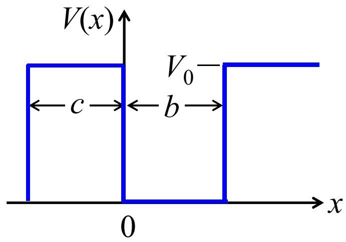
- Kronig-Penny model
- Tight-binding model
- Nearly free electron model

Kronig-Penny Model: Periodic Potential

- One electron approximation: Each valence electron is considered independent and only acted upon by the periodic positive ions.



Schrodinger's Equation



$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi(x)=\varepsilon\psi(x)$$

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}\left[\varepsilon-V(x)\right]\psi(x)=0$$

- Wavefunction will be of Bloch form: $\psi(x)=e^{ikx}u(x)$

  $\rightarrow$ $u(x)$ has the periodicity of the lattice.

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Schrodinger's Equation

- After substitution

$$\frac{d^2}{dx^2}e^{ikx}u(x)+\frac{2m}{\hbar^2}\left[\varepsilon-V(x)\right]e^{ikx}u(x)=0$$

$$\frac{d}{dx}\left[ike^{ikx}u(x)+e^{ikx}\frac{du(x)}{dx}\right]+\frac{2m}{\hbar^2}\left[\varepsilon-V(x)\right]e^{ikx}u(x)=0$$

$$\left(ik\right)^2 e^{ikx}u(x)+ike^{ikx}\frac{du(x)}{dx}+ike^{ikx}\frac{du(x)}{dx}+e^{ikx}\frac{d^2u(x)}{dx^2}$$

$$+\frac{2m}{\hbar^2}\left[\varepsilon-V(x)\right]e^{ikx}u(x)=0$$

$$\frac{d^2u(x)}{dx^2}+2ik\frac{du(x)}{dx}-k^2u(x)+\frac{2m}{\hbar^2}\left[\varepsilon-V(x)\right]u(x)=0$$

$$\frac{d^2u(x)}{dx^2}+2ik\frac{du(x)}{dx}-\left[k^2-\alpha^2+\frac{2mV(x)}{\hbar^2}\right]u(x)=0,\quad \alpha^2=\frac{2m\varepsilon}{\hbar^2}$$

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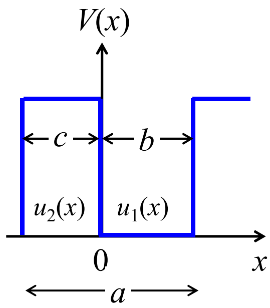
Potential Well and Barrier

$$\frac{d^2u(x)}{dx^2} + 2ik\frac{du(x)}{dx} - \left[k^2 - \alpha^2 + \frac{2mV(x)}{\hbar^2}\right]u(x) = 0$$



$0 < x < b:$

$$\frac{d^2u_1(x)}{dx^2} + 2ik\frac{du}{dx} - \left(k^2 - \alpha^2\right)u_1(x) = 0$$

$-c < x < 0:$

$$\frac{d^2u_2(x)}{dx^2} + 2ik\frac{du}{dx} - \left(k^2 - \beta^2\right)u_2(x) = 0$$

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

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Solutions

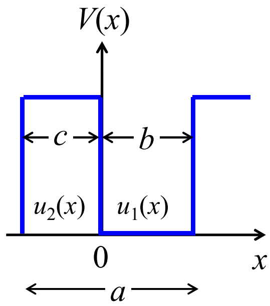
$0 < x < b:$

$$u_1(x) = Ae^{i(\alpha - k)x} + Be^{-i(\alpha + k)x}$$

$-c < x < 0:$

$$u_2(x) = Ce^{i(\beta - k)x} + De^{-i(\beta + k)x}$$

A, B, C, D are constants and must be determined.



Apply Boundary Conditions:

Wavefunctions and their derivatives must be continuous at all points.

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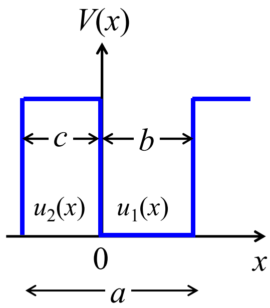
Boundary Conditions

- At $x = 0$

$$u_1(0) = u_2(0)$$

$$\Rightarrow \quad A + B = C + D$$



$$\left.\frac{du_1(x)}{dx}\right|_{x=0} = \left.\frac{du_2(x)}{dx}\right|_{x=0}$$

$$\Rightarrow \quad i(\alpha - k)A - i(\alpha + k)B = i(\beta - k)C - i(\beta + k)D$$

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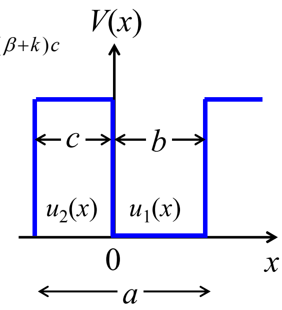
Boundary Conditions

- At $x = b$

$$u_1(b) = u_2(-c)$$

$$\Rightarrow \quad Ae^{i(\alpha-k)b} + Be^{-i(\alpha+k)b} = Ce^{-i(\beta-k)c} + De^{i(\beta+k)c}$$



$$\left.\frac{du_1(x)}{dx}\right|_{x=b} = \left.\frac{du_2(x)}{dx}\right|_{x=-c}$$

$$\Rightarrow \quad i(\alpha - k)Ae^{i(\alpha-k)b} - i(\alpha + k)Be^{-i(\alpha+k)b}$$
$$= i(\beta - k)Ce^{-i(\beta-k)c} - i(\beta + k)De^{i(\beta+k)c}$$

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Solutions

$$A+B=C+D$$
$$i(\alpha-k)A-i(\alpha+k)B=i(\beta-k)C-i(\beta+k)D$$
$$Ae^{i(\alpha-k)b}+Be^{-i(\alpha+k)b}=Ce^{-i(\beta-k)c}+De^{i(\beta+k)c}$$
$$i(\alpha-k)Ae^{i(\alpha-k)b}-i(\alpha+k)Be^{-i(\alpha+k)b}=i(\beta-k)Ce^{-i(\beta-k)c}-i(\beta+k)De^{i(\beta+k)c}$$

- For meaningful solutions to exist, the determinant must be zero:

$$\begin{vmatrix} 1 & 1 & 1 & 1 \\ \alpha-k & -(\alpha+k) & \beta-k & -(\beta+k) \\ e^{i(\alpha-k)b} & e^{-i(\alpha+k)b} & e^{-i(\beta-k)c} & e^{i(\beta+k)c} \\ (\alpha-k)e^{i(\alpha-k)b} & -(\alpha+k)e^{-i(\alpha+k)b} & (\beta-k)e^{-i(\beta-k)c} & -(\beta+k)e^{i(\beta+k)c} \end{vmatrix}=0$$

Dispersion Relation

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

$\beta^2>0 \rightarrow \beta$ is real.

$$-\frac{\alpha^2+\beta^2}{2\alpha\beta}\sin\alpha b\sin\beta c+\cos\alpha b\cos\beta c=\cos ka$$

$\beta^2<0 \rightarrow \beta$ is imaginary.

$$\frac{\gamma^2-\alpha^2}{2\alpha\gamma}\sin\alpha b\sinh\gamma c+\cos\alpha b\cosh\gamma c=\cos ka$$

$$\beta=i\gamma$$

Dispersion Relation

- Using trigonometry

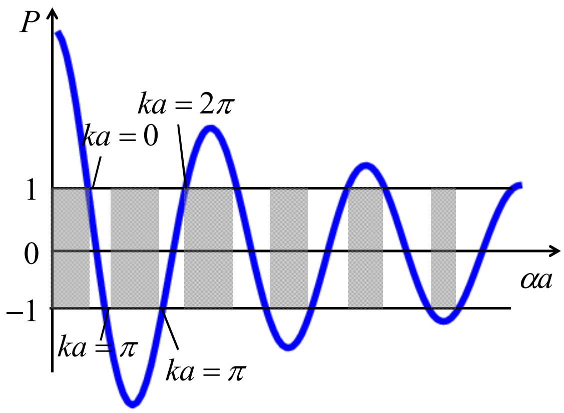
$$\left[1+\frac{V_0^2}{4\varepsilon(\varepsilon-V_0)}\sin^2\beta c\right]^{1/2}\cos(\alpha b-\delta)=\cos ka, \qquad (\varepsilon>V_0)$$

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

where

$$\tan\delta=-\frac{\alpha^2+\beta^2}{2\alpha\beta}\tan\beta c \quad \text{and} \quad \tan\delta'=\frac{\gamma^2-\alpha^2}{2\alpha\gamma}\tanh\gamma c$$

Energy Bands



Forbidden energy range

$$\alpha^2=\frac{2m\varepsilon}{\hbar^2}$$

- 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 $2N$ states for spin degeneracy.
- The energy gaps decrease as electron energy increases → free electron behavior at high energies.