Intro. to Electro-physics

The band theory and semiconductors (I)

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Free vs. nearly-free electron models (1/2)

- **Free electron model**
  - **can** explain limited aspects of heat capacity, thermal conductivity, electrical conductivity and etc.
  - **cannot** predict the positive Hall coefficient and many detailed transport properties
  - **cannot** distinguish between metals, semiconductors and insulators

- **Nearly-free electron model**
  - Electrons move nearly freely, while being subject to **a weak, periodic potential** due to the periodic lattice

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx} + V(x)\psi(x) = E\psi(x), \text{ where } V(x+na) = V(x)$$

  - Solution $\psi(x)$: **Bloch's state**
  - The most important property of solids, **"allowed bands"** and **"forbidden gaps"**, emerges as a result!
    - Metal: one more more bands are partly filled
    - Insulator: bands are either completely empty or filled
    - Semiconductor: one or two bands are slightly filled or slightly empty

Free vs. nearly-free electron models (2/2)

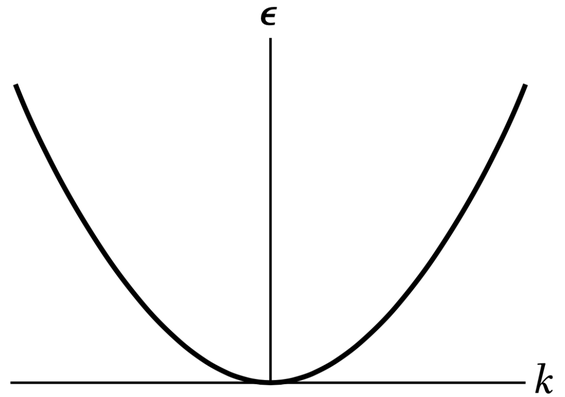
- **Free electron model**
  - Dispersion relation $\left(\varepsilon \text{ vs. } \boldsymbol{k}\right)$

$$\varepsilon_{\boldsymbol{k}} = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right), \text{ where } \left(k_x, k_y, k_z\right) = 0, \pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}, \cdots$$

  - Wave function for a free electron

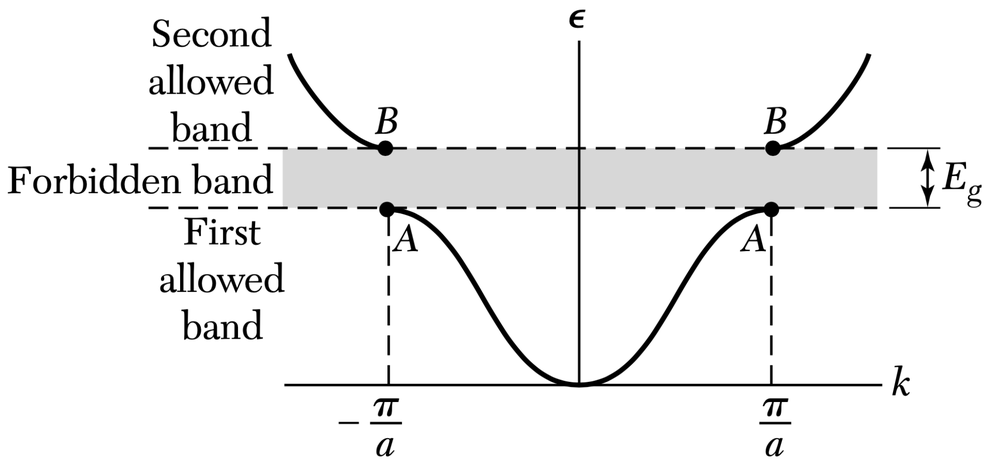
$$\psi_{\boldsymbol{k}} = \exp\left(i\boldsymbol{k}\cdot\boldsymbol{r}\right)$$

    : Traveling wave that carries a momentum $\boldsymbol{p} = \hbar\boldsymbol{k}$



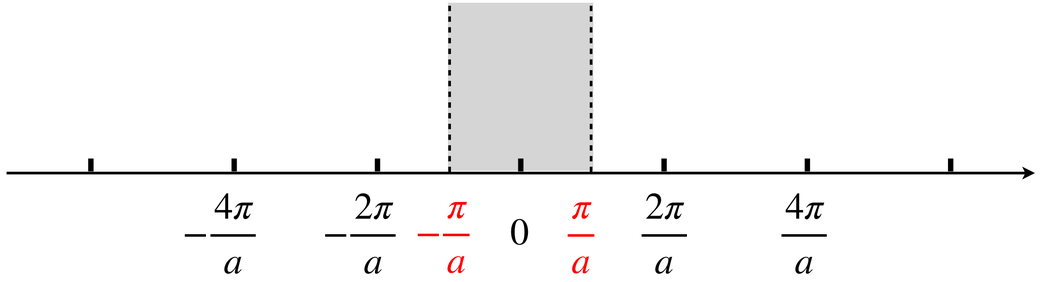
Free electron model

- **Nearly-free electron model**
  - The electrons in crystals perturbed “only weakly” by the **periodic potential** of the ion cores
  - **Bragg reflection** at Brillouin zone boundary occurs
    - a characteristic feature of wave propagation in crystals
    - the cause of **energy gaps**



Nearly-free electron model

Origin of a band gap (1/2)



- 1D model
  - The Bragg condition in 1D

$$2\boldsymbol{k}\cdot\boldsymbol{G}=G^2 \longrightarrow \boxed{k=\pm\frac{1}{2}G=\pm\frac{n\pi}{a},\ \text{where } G=\frac{2\pi n}{a}\ \text{: a reciprocal lattice vector}}$$

  - The first Brillouin zone in k-space = $\left[-\pi/a,\pi/a\right]$
  - At zone boundaries $\left(k=\pm\pi/a\right)$
    - A wave traveling to the right is Bragg-reflected to travel to the left, and vice versa
    - Two waves traveling to the left & right :

$$\exp\left(\pm i\frac{\pi x}{a}\right)=\cos\left(\frac{\pi x}{a}\right)\pm i\sin\left(\frac{\pi x}{a}\right)$$

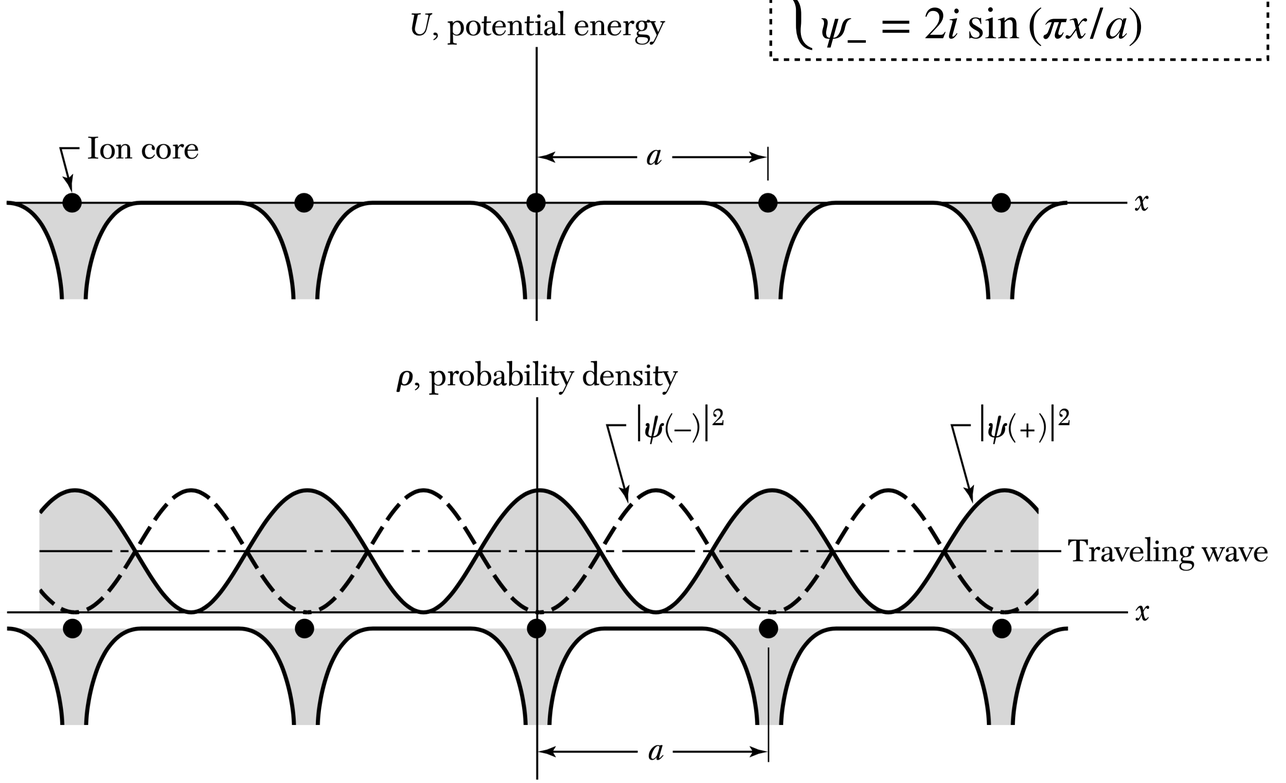
    - Two standing waves are resulted :

$$\begin{cases}\psi_+=\exp\left(i\pi x/a\right)+\exp\left(-i\pi x/a\right)=2\cos\left(\pi x/a\right)\\ \psi_-=\exp\left(i\pi x/a\right)-\exp\left(-i\pi x/a\right)=2i\sin\left(\pi x/a\right)\end{cases}$$

Origin of a band gap (2/2)

Waves at the zone boundary

$$\begin{cases} \psi_+ = 2\cos(\pi x/a) \\ \psi_- = 2i\sin(\pi x/a) \end{cases}$$



- Probability density of a wave-like particle

$$\rho = \left|\psi\right|^2 = \psi^*\psi$$

  - Probability density for a traveling wave

$$\rho_0 = \exp\left(-ikx\right)\exp\left(ikx\right) = 1$$

  - Probability density for waves in crystals

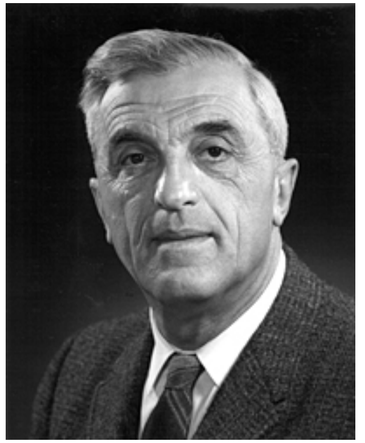
$$\begin{cases} \rho_+ = \left|\psi_+\right|^2 \propto \cos^2(\pi x/a) \\ \rho_- = \left|\psi_-\right|^2 \propto \sin^2(\pi x/a) \end{cases}$$

    - ρ_+ piles up electrons on the positive ions, where the potential energy is lowest
    - ρ_- concentrates electrons away from the ion cores

  - **The average of the potential energy & energy gap**

$$U_{\rho_+} < U_{\rho_0} < U_{\rho_-} \text{ and } U_{\rho_-} - U_{\rho_+} \triangleq E_g$$

Bloch theorem



Felix Bloch
(Switzerland)
1905-1983

- Bloch theorem
  - The solutions of the Schrödinger equation for a periodic potential is given in a form :

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = u_{\boldsymbol{k}}(\boldsymbol{r}) \exp\left(i\boldsymbol{k}\cdot\boldsymbol{r}\right), \text{ where } u_{\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{T}) = u_{\boldsymbol{k}}(\boldsymbol{r})$$

    - $u_{\boldsymbol{k}}(\boldsymbol{r})$: a periodic function
    - $\boldsymbol{T} = v_1\boldsymbol{a}_1 + v_1\boldsymbol{a}_2 + v_1\boldsymbol{a}_3$: Translation vector of a lattice
    - $\exp\left(i\boldsymbol{k}\cdot\boldsymbol{r}\right)$: propagation (with an oscillation strength and direction)

  - Probability of finding an electron at $\boldsymbol{r}$

$$P_{\boldsymbol{k}}(\boldsymbol{r}) = \left|\psi_{\boldsymbol{k}}(\boldsymbol{r})\right|^2 = \left|u_{\boldsymbol{k}}(\boldsymbol{r})\exp\left(i\boldsymbol{k}\cdot\boldsymbol{r}\right)\right|^2 = \left|u_{\boldsymbol{k}}(\boldsymbol{r})\right|^2 \quad \left(\because \left|\exp\left(i\boldsymbol{k}\cdot\boldsymbol{r}\right)\right| = 1\right)$$

$$\therefore P_{\boldsymbol{k}}(\boldsymbol{r}+\boldsymbol{T}) = P_{\boldsymbol{k}}(\boldsymbol{r})$$

    - Probability of finding an electron at $\boldsymbol{r}$ in the unit cell = that in “every” cell of the whole crystal
    - Such electronic state = Bloch’s state = Delocalized state

1D model for a band structure (1/3)

- Simple 1D Dirac-comb model
  - Schrödinger's equation with a periodic potential $V(x)$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi, \text{ where } V(x+a) = V(x)$$

  - 1D Dirac-comb potential

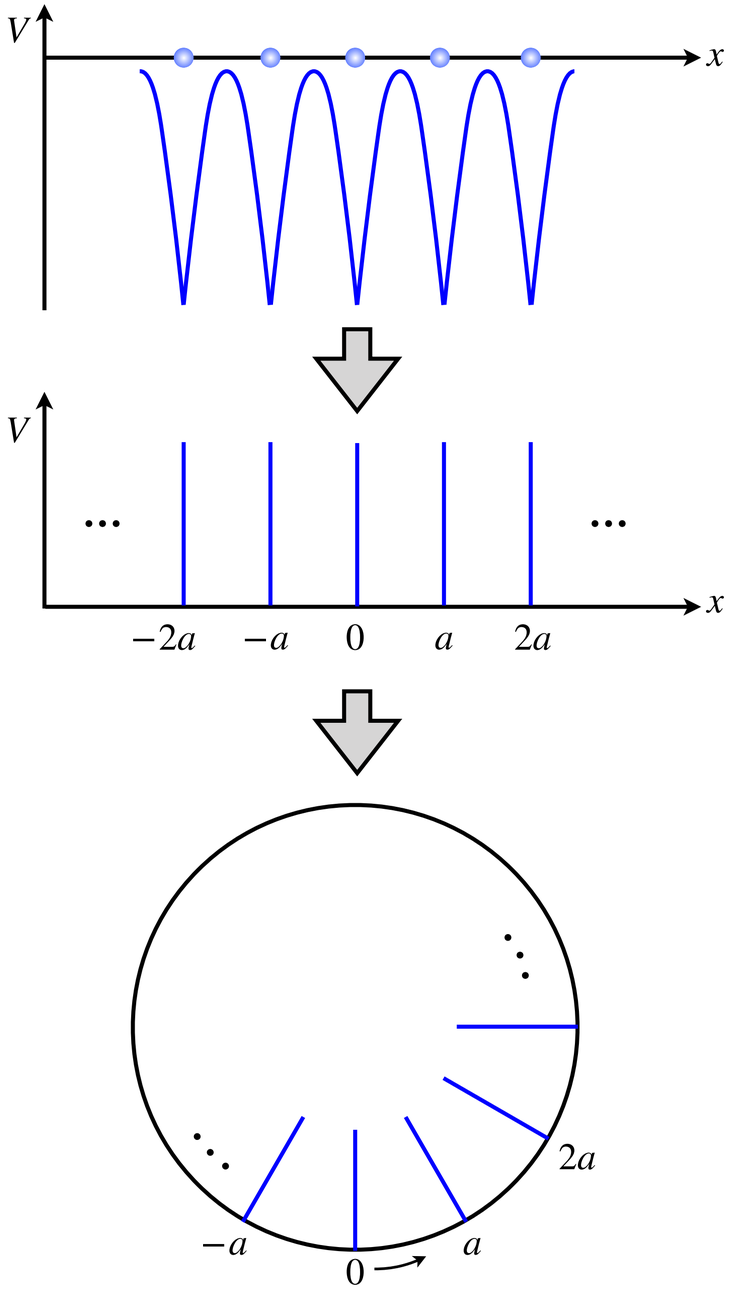
$$V(x) = \alpha \sum_{j=0}^{N-1} \delta\left(x - ja\right)$$

  - Periodic boundary condition (ring-shaped)

$$\psi(x + Na) = \psi(x), \ \left(N > 10^{23}\text{cm}^{-3} : \text{number of atoms}\right)$$

  - Bloch's theorem in 1D

$$\psi(x + a) = e^{iqa}\psi(x) \quad \text{(for some constant } q\text{)}$$



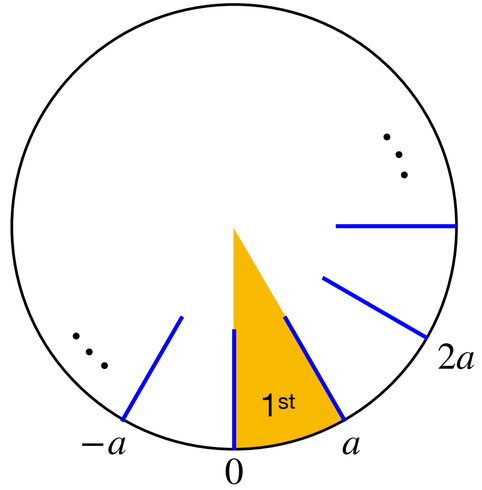
1D model for a band structure (2/3)

$\psi(x+Na) = \psi(x)$: B.C.

$\psi(x+a) = e^{iqa}\psi(x)$: Bloch's theorem

- Simple 1D Dirac-comb model (contd.)
  - By combining Bloch's theorem & periodic boundary condition,
    - $\left[\psi(x+Na) = e^{iqNa}\psi(x)\right] = \psi(x)$
    - $e^{iqNa} = 1 \longrightarrow qNa = 2\pi n$

$$\therefore q = \frac{2\pi n}{Na}, \quad (n = 0, \pm 1, \pm 2, \cdots)$$



- (revisited) Schrödinger's equation
  - Wavefunction within the 1st unit cell $(0 < x < a)$ where $V(x) = 0$
    - $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \longrightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$
    - $\frac{d^2\psi}{dx^2} = -k^2\psi$, where $k = \frac{\sqrt{2mE}}{\hbar}$
    - $\psi(x) = A\sin(kx) + B\cos(kx), \quad (0 < x < a)$

1D model for a band structure (3/3)

Wavefunction in the 1st unit cell

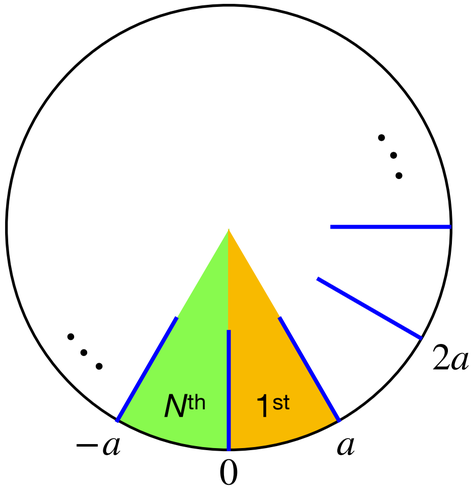
$$\psi(x) = A\sin(kx) + B\cos(kx)$$

- Schrödinger's equation (revisited)
  - wavefunction for the N^{th} cell immediately to the left of the origin:

$$\psi(x-a) = e^{-iqa}\psi(x), \quad (0 < x < a) \quad (\because \text{Bloch's theorem})$$

▶ Let $x' \triangleq x - a$. Then,

$$\blacktriangleright\ \psi(x') = e^{-iqa}\left[A\sin q(x'+a) + B\cos k(x'+a)\right], \quad (-a < x' < 0)$$



- Boundary condition
  - $\psi(x)$ must be continuous at $x = 0$:

$$B = e^{-iqa}\left[A\sin(ka) + B\cos(ka)\right] \quad \cdots ①$$

  - $d\psi(x)/dx$ suffers a discontinuity due to the delta function :

$$kA - e^{-iqa}k\left[A\cos(ka) - B\sin(ka)\right] = \frac{2m\alpha}{\hbar^2}B \quad \cdots ②$$

$$\cos(qa) = \cos(ka) + \frac{m\alpha}{\hbar^2 k}\sin(ka)$$

- It is a function of k
- It determines the possible values of k and associated energies! $\left(\because E = \hbar^2 k^2/2m\right)$

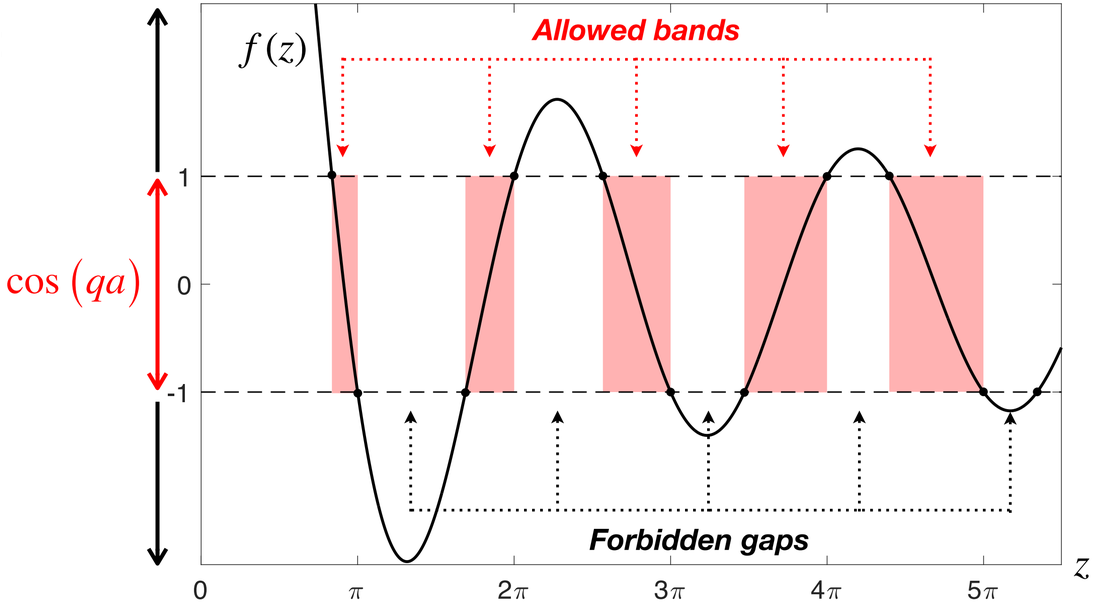
Band structure (1/2)

- Band structure
  - Solution to Schrödinger's equation for a periodic potential :

$$\cos(qa) = \cos(ka) + \frac{m\alpha}{\hbar^2 k}\sin(ka), \text{ where } q = \frac{2\pi n}{Na}$$

  - For simplicity, let $ka \triangleq z$ and $\frac{m\alpha a}{\hbar^2} \triangleq \beta$

$$\left[\cos(qa) = \cos\left(\frac{2\pi n}{N}\right)\right] = \left[\cos z + \beta\frac{\sin z}{z} \triangleq f(z)\right]$$



    - $\left|\cos\left(\frac{2\pi n}{N}\right)\right| \leq 1$: The region where solutions exist **(allowed band)**
    - $\left|\cos\left(\frac{2\pi n}{N}\right)\right| > 1$: The region with no solutions **(forbidden gap)**

Band structure (2/2)

- Band structure
  - Allowed band
    - Intercepts between N horizontal lines and $f(z) \rightarrow N$ solutions
    - In each band, there are closely spaced N electronic states
    - Since $N \gg 10^{23}$ (cm^3), a continuum of N electronic states = Band
  - Band structure = alternating bands and gaps
  - Band structure = a signature of a periodic potential
- Ground state of multi-electrons atomic crystal
  - Each state can accommodate 2 electrons (∵Exclusion principle)
  - d : the number of valence electrons per atom
    - $d = 1$: Half fill the first band
    - $d = 2$: Completely fill the first band
    - $d = 3$: Half fill the second band
    - …and so on