Task 1: Band gap dependence on potential height V_0

1.1 Kronig-Penney Model Fundamentals

We consider a 1D periodic potential with period $L = a + b$:

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < a \text{(well region)} \\ V_0 & \text{for } a < x < L \text{(barrier region)} \end{cases}$$

The time-independent Schrödinger equation:

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

In the well region (0 < x < a), V = 0:

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0, \alpha = \sqrt{\frac{2mE}{\hbar^2}}$$

Solution: $\psi(x) = A\cos(\alpha x) + B\sin(\alpha x)$

In the barrier region (a < x < L), V = V_0:

$$\frac{d^2\psi}{dx^2} - \beta^2\psi = 0, \beta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Solution: $\psi(x) = C\cosh(\beta x) + D\sinh(\beta x)$

1.2 Boundary Conditions and Transfer Matrix

Using continuity of ψ and dψ/dx at x = a and Bloch periodicity ψ(x+L) = e^{ikL}ψ(x), we derive the central equation:

$$\cos(kL) = \cos(\alpha a)\cosh(\beta b) + \frac{\beta^2 - \alpha^2}{2\alpha\beta}\sin(\alpha a)\sinh(\beta b)$$

This is the **Kronig-Penney equation**.

1.3 Band Gap at Brillouin Zone Boundary

The Brillouin zone boundaries occur at $k = \frac{n\pi}{L}$. For the first gap, n = 1: $k = \frac{\pi}{L}$.

At these points, the left side: $\cos(kL) = \cos(\pi) = -1$

The band edges occur when the right side equals ±1. The gap appears when the right side cannot satisfy the equation for real k.

1.4 Perturbation Theory Approach

For weak potentials (V_0 small), we can use nearly-free electron approximation.

The Fourier component for reciprocal vector $G = \frac{2\pi}{L}$:

$$V_G = \frac{1}{L}\int_0^L V(x)e^{-iGx}dx = \frac{1}{L}\left[\int_0^a 0 \cdot e^{-iGx}dx + \int_a^L V_0 e^{-iGx}dx\right]$$

$$V_G = \frac{V_0}{L}\int_a^L e^{-iGx}dx = \frac{V_0}{L}\left[\frac{e^{-iGx}}{-iG}\right]_a^L$$

$$V_G = \frac{V_0}{-iGL}(e^{-iGL} - e^{-iGa})$$

Since $G = \frac{2\pi}{L}$, then $GL = 2\pi$, so $e^{-iGL} = e^{-i2\pi} = 1$:

$$V_G = \frac{V_0}{-iGL}(1 - e^{-iGa})$$

Now compute Ga:

$$G = \frac{2\pi}{L} = \frac{2\pi}{a+b} = \frac{2\pi}{2.5\ \text{Å}} \text{(but we only need the phase)}$$
$$Ga = \frac{2\pi a}{a+b} = \frac{2\pi \times 1.5}{2.5} = 1.2\pi = 216^\circ$$

Thus:

$$V_G = \frac{V_0}{-iGL}(1 - e^{-i1.2\pi})$$

Magnitude:

$$| V_G | = \frac{V_0}{GL} | 1 - e^{-i1.2\pi} | = \frac{V_0}{2\pi}\sqrt{(1 - \cos(1.2\pi))^2 + (\sin(1.2\pi))^2}$$

Compute trigonometric values:

$$\cos(1.2\pi) = \cos(216^\circ) = -\cos(36^\circ) \approx -0.8090$$
$$\sin(1.2\pi) = \sin(216^\circ) = -\sin(36^\circ) \approx -0.5878$$

Then:

$$| 1 - e^{-i1.2\pi} | = \sqrt{(1 - (-0.8090))^2 + (-0.5878)^2} = \sqrt{(1.8090)^2 + (0.5878)^2}$$
$$= \sqrt{3.2725 + 0.3455} = \sqrt{3.6180} \approx 1.9021$$

Therefore:

$$| V_G | = \frac{V_0}{2\pi} \times 1.9021 \approx 0.3027 V_0$$

1.5 Band Gap Expression

In nearly-free electron model, the band gap at BZ boundary is:

$$E_g = 2 | V_G | \approx 2 \times 0.3027 V_0 = 0.6054 V_0$$

1.6 Detailed Dependence and Saturation

For small V_0: $E_g \propto V_0$

For large V_0, the gap approaches the difference between the first two energy levels of an isolated well of width a:

In an infinite square well of width a:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

$$E_2 - E_1 = \frac{(4-1)\pi^2\hbar^2}{2ma^2} = \frac{3\pi^2\hbar^2}{2ma^2}$$

With a = 1.5 Å = 1.5×10^{-10} m:

$$\frac{\hbar^2}{2m} \approx 3.81 \times 10^{-20}$$

$$E_2 - E_1 = \frac{3\pi^2 \times 3.81 \times 10^{-20}}{(2.25 \times 10^{-20})} \approx \frac{3 \times 9.87 \times 3.81}{2.25} \approx 50.2\,\text{eV}$$

So saturation occurs around 50 eV, but for V_0 = 0-10 eV, we're in the linear regime.

Task 2: Band gap dependence on barrier width b

2.1 Modified Fourier Component

Now a = 1.5 Å fixed, V_0 = 5 eV fixed, b variable, L = a + b.

The potential is now:

$$V(x) = \begin{cases} V_0 & \text{for } 0 < x < b \text{(barrier first)} \\ 0 & \text{for } b < x < L \text{(well)} \end{cases}$$

But due to periodicity, we can shift the origin. The Fourier component:

$$V_G = \frac{1}{L}\int_0^L V(x)e^{-iGx}dx = \frac{1}{L}\left[\int_0^b V_0 e^{-iGx}dx + \int_b^L 0 \cdot e^{-iGx}dx\right]$$

$$V_G = \frac{V_0}{L}\int_0^b e^{-iGx}dx = \frac{V_0}{L}\left[\frac{e^{-iGx}}{-iG}\right]_0^b = \frac{V_0}{-iGL}(e^{-iGb} - 1)$$

Magnitude:

$$|\,V_G\,| = \frac{V_0}{GL}\,|\,e^{-iGb} - 1\,| = \frac{V_0}{GL}\,|\,1 - e^{-iGb}\,|$$

Since $G = \frac{2\pi}{L}$, $GL = 2\pi$:

$$|\,V_G\,| = \frac{V_0}{2\pi} \cdot 2\,|\,\sin\left(\frac{Gb}{2}\right)\,| = \frac{V_0}{\pi}\,|\,\sin\left(\frac{Gb}{2}\right)\,|$$

But $\frac{Gb}{2} = \frac{\pi b}{L}$, so:

$$|\,V_G\,| = \frac{V_0}{\pi}\,|\,\sin\left(\frac{\pi b}{L}\right)\,| = \frac{V_0}{\pi}\,|\,\sin\left(\frac{\pi b}{a+b}\right)\,|$$

2.2 Band Gap Expression

$$E_g \approx 2\,|\,V_G\,| = \frac{2V_0}{\pi}\,|\,\sin\left(\frac{\pi b}{a+b}\right)\,|$$

2.3 Analysis of the Sine Function

Let $f(b) = |\,\sin\left(\frac{\pi b}{a+b}\right)\,|$

- When b = 0: f(0) = |sin(0)| = 0 → E_g = 0
- When b → ∞: f(∞) = |sin(π)| = 0 → E_g = 0
- Maximum when $\frac{\pi b}{a+b} = \frac{\pi}{2} \Rightarrow \frac{b}{a+b} = \frac{1}{2} \Rightarrow$ b = a

At b = a = 1.5 Å:

$$f_{max} = |\sin(\frac{\pi \times 1.5}{3.0})| = |\sin(\pi/2)| = 1$$

$$E_g^{max} = \frac{2 \times 5}{\pi} \times 1 = \frac{10}{\pi} \approx 3.183 \text{ eV}$$

2.4 Detailed Function Behavior

Let's compute sample values:

For b = 0.5 Å: $\frac{b}{a+b} = \frac{0.5}{2.0} = 0.25$, sin(0.25π) = sin(45°) ≈ 0.7071

E_g ≈ (10/π)×0.7071 ≈ 2.25 eV

For b = 1.0 Å: $\frac{1.0}{2.5} = 0.4$, sin(0.4π) = sin(72°) ≈ 0.9511

E_g ≈ 3.03 eV

For b = 1.5 Å: $\frac{1.5}{3.0} = 0.5$, sin(π/2) = 1

E_g ≈ 3.18 eV

For b = 2.0 Å: $\frac{2.0}{3.5} \approx 0.571$, sin(0.571π) = sin(102.9°) ≈ 0.9749

E_g ≈ 3.10 eV

For b = 3.0 Å: $\frac{3.0}{4.5} \approx 0.667$, sin(0.667π) = sin(120°) ≈ 0.8660

E_g ≈ 2.76 eV

Task 3: Amorphous solids and band gaps - Detailed Analysis

3.1 Mathematical Foundation of Band Gaps in Periodic Systems

The band gap arises from the solution of the Schrödinger equation with periodic potential:

$$[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})]\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

For periodic potential: $V(\mathbf{r} + \mathbf{R}) = V(\mathbf{r})$ for all Bravais lattice vectors **R**

Bloch's theorem: $\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r})$

The band gap emerges from the **band structure equation**:

$$E_n(\mathbf{k}) = \frac{\hbar^2}{2m}|\mathbf{k} + \mathbf{G}|^2 + \sum_{\mathbf{G}'} V_{\mathbf{G}'} c_{\mathbf{k}+\mathbf{G},\mathbf{G}'}$$

where the gap at Brillouin zone boundary is approximately $2|V_G|$.

3.2 Short-Range Order Parameters

In amorphous materials, we lack long-range periodicity but retain **short-range order** characterized by:

Radial distribution function $g(r)$:

$$g(r) = \frac{1}{N\rho}\sum_{i \neq j} \langle \delta(r - |\mathbf{r}_i - \mathbf{r}_j|) \rangle$$

Structure factor $S(\mathbf{q})$:

$$S(\mathbf{q}) = 1 + \rho \int [g(r) - 1] e^{-i\mathbf{q}\cdot\mathbf{r}} d^3r$$

For amorphous materials, $S(\mathbf{q})$ shows broad peaks at q_0 corresponding to inverse interatomic spacing.

3.3 Effective Potential in Amorphous Systems

The potential can be expressed as:

$$V(\mathbf{r}) = \sum_i \quad v(|\ \mathbf{r} - \mathbf{R}_i\ |)$$

where $v(r)$ is the atomic potential. The Fourier transform:

$$V(\mathbf{q}) = v(\mathbf{q}) S(\mathbf{q})$$

The **pseudogap** appears when:

$$|\ V(q_0)\ | \geq \frac{\hbar^2 q_0^2}{8m}$$

where q_0 is the position of the first peak in $S(q)$.

3.4 Quantitative Analysis from Tasks 1 & 2

From Task 1: $E_g \propto V_0 \rightarrow$ **Atomic potential strength** matters

- For SiO_2: Strong ionic potential (Z_Si = 14, Z_O = 8) → large V_0
- Coulomb potential: $v(r) \propto \frac{Ze^2}{r}$ → large Z gives deep potential wells

From Task 2: $E_g \propto |\ \sin\left(\frac{\pi b}{a+b}\right)\ | \rightarrow$ **Spatial arrangement** matters

- In amorphous materials: $a \approx$ average bond length
- For SiO_2: Si-O bond length ≈ 1.6 Å determines effective well width

3.5 Coordination and Bond Angle Effects

The **local coordination number** N_c affects the potential shape:

For tetrahedral coordination (SiO_2):

- Bond angle distribution centered at ≈ 109°
- Creates well-defined local potential minima

The **order parameter** for short-range order:

$$Q_l = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} \quad |\ Q_{lm}\ |^2, Q_{lm} = \frac{1}{N} \sum_i \quad Y_{lm}(\theta_i, \phi_i)$$

where Y_{lm} are spherical harmonics.

3.6 Mathematical Criterion for Band Gap Formation

A band gap forms when the **Ioffe-Regel criterion** is satisfied:

$$k_F l_e \lesssim 1$$

where k_F is Fermi wavevector and l_e is electron mean free path.

In amorphous materials, the **Anderson localization** condition:

$$\frac{V_0}{W} \gtrsim \frac{\pi}{2\sqrt{3}} \approx 0.91$$

where V_0 is disorder strength and W is bandwidth.
For SiO_2: V_0 (ionic potential) ≈ 20 eV, W ≈ 10 eV → ratio ≈ 2 ≫ 0.91 → strong localization → clear band gap.

Task 4: Bragg law and electron behavior - Rigorous Treatment

4.1 Derivation of Bragg Law from Wave Interference

Consider waves incident on crystal planes with spacing d. Path difference between waves scattered from adjacent planes:

$$\Delta = AB + BC = d\sin\,\theta + d\sin\,\theta = 2d\sin\,\theta$$

Constructive interference when:

$$2d\sin\,\theta = n\lambda, n \in \mathbb{Z}$$

4.2 Electron Waves and Reciprocal Space

For electrons: $\lambda = \frac{2\pi}{k}$, so Bragg condition becomes:

$$2d\sin\,\theta = n\frac{2\pi}{k} \Rightarrow k\sin\,\theta = \frac{n\pi}{d}$$

For normal incidence ($\theta = 90°$):

$$k = \frac{n\pi}{d}$$

4.3 Brillouin Zone Construction

Reciprocal lattice vectors: $\mathbf{G} = \frac{2\pi}{d}\mathbf{n}$

First Brillouin zone boundary: $k = \frac{\pi}{d}$

The Bragg condition is equivalent to:

$$|\,\mathbf{k}\,| = |\,\mathbf{k} + \mathbf{G}\,|$$

which defines the Brillouin zone boundaries.

4.4 Detailed Analysis at Zone Boundary

At $k = \frac{\pi}{d}$, the electron waves satisfy:

$$\psi_+ = e^{i\pi x/d} + e^{-i\pi x/d} = 2\cos\,(\frac{\pi x}{d})$$

$$\psi_- = e^{i\pi x/d} - e^{-i\pi x/d} = 2i\sin\,(\frac{\pi x}{d}) Thesestandingwaveshavedifferentcharge$$

$$\rho_-(x) = |\,\psi_-\,|^2 \propto \sin^2(\frac{\pi x}{d})$$

The electrostatic energy difference:

$$\Delta E = \int V(x)[\rho_+(x) - \rho_-(x)]dx$$

For periodic potential $V(x) = V_0 \cos(2\pi x/d)$:

$$\Delta E = V_0 \int_0^d \cos(\frac{2\pi x}{d})[\cos^2(\frac{\pi x}{d}) - \sin^2(\frac{\pi x}{d})]dx$$

Using $\cos^2\theta - \sin^2\theta = \cos 2\theta$:

$$\Delta E = V_0 \int_0^d \cos(\frac{2\pi x}{d})\cos(\frac{2\pi x}{d})dx = V_0 \int_0^d \cos^2(\frac{2\pi x}{d})dx = \frac{V_0 d}{2}$$

Thus the band gap: $E_g = \Delta E = \frac{V_0 d}{2}$

4.5 Electron Behavior Away from Zone Boundary

For $k \ll \frac{\pi}{d}$, use **perturbation theory**:

Unperturbed energy: $E^{(0)}(k) = \frac{\hbar^2 k^2}{2m}$

First-order correction: $E^{(1)}(k) = \langle k \mid V \mid k \rangle = V_0 \delta_{G,0} = 0$

Second-order correction:

$$E^{(2)}(k) = \sum_{G \neq 0} \frac{|\langle k \mid V \mid k+G \rangle|^2}{E^{(0)}(k) - E^{(0)}(k+G)}$$

For small k, denominator $\approx -\frac{\hbar^2 G^2}{2m}$, so:

$$E^{(2)}(k) \approx -\frac{2m \mid V_G \mid^2}{\hbar^2 G^2}$$

Thus the energy is lowered by a constant amount, and the effective mass becomes:

$$\frac{m^*}{m} = [1 + \frac{2m \mid V_G \mid^2}{\hbar^2 G^2 E^{(0)}(G)}]^{-1}$$

Task 5: Empty lattice model in 1D - Complete Derivation

5.1 Mathematical Foundation

We solve: $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$ with Bloch boundary conditions: $\psi(x+a) = e^{ika}\psi(x)$

General solution: $\psi(x) = Ae^{iKx}$, where $K = k + G_n$, $G_n = \frac{2\pi n}{a}$

Energy: $E(K) = \frac{\hbar^2}{2m}K^2$

5.2 Reduced Zone Scheme Construction

We map all K to the first Brillouin zone: $-\frac{\pi}{a} < k \leq \frac{\pi}{a}$

For each n, define: $k = K - G_n$, with k in 1st BZ

Then: $E_n(k) = \frac{\hbar^2}{2m}(k + G_n)^2$

5.3 Explicit Band Calculations

Let $E_0 = \frac{\hbar^2}{2m}(\frac{\pi}{a})^2$ be the energy unit.

Band 1 (n = 0):

$$E_0(k) = \frac{\hbar^2}{2m}k^2 = E_0(\frac{k}{\pi/a})^2$$

Band 2 (n = -1):

$$G_{-1} = -\frac{2\pi}{a}, E_{-1}(k) = \frac{\hbar^2}{2m}(k - \frac{2\pi}{a})^2$$

Band 3 (n = 1):

$$G_1 = \frac{2\pi}{a}, E_1(k) = \frac{\hbar^2}{2m}(k + \frac{2\pi}{a})^2$$

5.4 Detailed Band Values

Let $\kappa = \frac{k}{\pi/a}$, so $\kappa \in (-1,1]$

Band 1: $E_0(\kappa) = E_0\kappa^2$

Band 2: $E_{-1}(\kappa) = E_0(\kappa - 2)^2$

Band 3: $E_1(\kappa) = E_0(\kappa + 2)^2$

At specific points:

At $\kappa = 0$ (Γ point):

- $E_0 = 0$
- $E_{-1} = E_0(0 - 2)^2 = 4E_0$
- $E_1 = E_0(0 + 2)^2 = 4E_0$

At $\kappa = 1$ (BZ boundary):

- $E_0 = E_0$
- $E_{-1} = E_0(1 - 2)^2 = E_0$
- $E_1 = E_0(1 + 2)^2 = 9E_0$

At $\kappa = -1$ (equivalent to $\kappa = 1$):

- $E_0 = E_0$
- $E_{-1} = E_0(-1 - 2)^2 = 9E_0$
- $E_1 = E_0(-1 + 2)^2 = E_0$

5.5 Wavefunction Derivation

Bloch theorem: $\psi_{nk}(x) = e^{ikx}u_{nk}(x)$, with $u_{nk}(x + a) = u_{nk}(x)$

For empty lattice, the periodic function is:

$$u_{nk}(x) = \frac{1}{\sqrt{a}}e^{iG_nx} = \frac{1}{\sqrt{a}}e^{i\frac{2\pi n}{a}x}$$

Thus:

$$\psi_{nk}(x) = \frac{1}{\sqrt{a}}e^{ikx}e^{i\frac{2\pi n}{a}x} = \frac{1}{\sqrt{a}}e^{i(k+\frac{2\pi n}{a})x}$$

Normalization: $\int_0^a \quad |\psi_{nk}(x)|^2\, dx = \frac{1}{a}\int_0^a \quad dx = 1$

5.6 Band Degeneracies

Degeneracies occur when $E_n(k) = E_m(k)$ for n ≠ m:

$$(k + G_n)^2 = (k + G_m)^2 \Rightarrow k + G_n = \pm(k + G_m)$$

Case 1: $k + G_n = k + G_m \Rightarrow G_n = G_m$ (impossible for n ≠ m)

Case 2: $k + G_n = -(k + G_m) \Rightarrow 2k = -G_n - G_m$

For n = 1, m = -1: $G_1 = \frac{2\pi}{a}, G_{-1} = -\frac{2\pi}{a}$

$$2k = -(\frac{2\pi}{a} - \frac{2\pi}{a}) = 0 \Rightarrow k = 0$$

Degeneracy at Γ point: $E_1(0) = E_{-1}(0) = 4E_0$

At BZ boundary ($k = \pi/a$): $E_0 = E_{-1} = E_0$

Task 6: 2D Square Lattice - Comprehensive Treatment

6.1 Reciprocal Space Geometry

Square lattice: primitive vectors $\mathbf{a}_1 = a\hat{x}, \mathbf{a}_2 = a\hat{y}$

Reciprocal lattice vectors:

$$\mathbf{b}_1 = \frac{2\pi}{a}\hat{x}, \mathbf{b}_2 = \frac{2\pi}{a}\hat{y}$$

General reciprocal vector:

$$\mathbf{G}_{mn} = m\mathbf{b}_1 + n\mathbf{b}_2 = \frac{2\pi}{a}(m, n)$$

6.2 High-Symmetry Points

X point: $\mathbf{k}_X = \frac{\pi}{a}(1,0)$

M point: $\mathbf{k}_M = \frac{\pi}{a}(1,1)$

Path X→M: $\mathbf{k} = \frac{\pi}{a}(1, \kappa)$, where κ goes from 0 to 1

6.3 Empty Lattice Bands

Energy expression:

$$E_{mn}(\mathbf{k}) = \frac{\hbar^2}{2m}|\mathbf{k} + \mathbf{G}_{mn}|^2 = \frac{\hbar^2}{2m}[(k_x + \frac{2\pi m}{a})^2 + (k_y + \frac{2\pi n}{a})^2]$$

Substitute $k_x = \frac{\pi}{a}, k_y = \frac{\pi}{a}\kappa$:

$$E_{mn}(\kappa) = \frac{\hbar^2}{2m}[(\frac{\pi}{a} + \frac{2\pi m}{a})^2 + (\frac{\pi\kappa}{a} + \frac{2\pi n}{a})^2]$$

6.4 Dimensionless Form

Let $E_0 = \frac{\hbar^2}{2m}(\frac{\pi}{a})^2$

Then:

$$E_{mn}(\kappa) = E_0[(1 + 2m)^2 + (\kappa + 2n)^2]$$

6.5 Specific Band Calculations

Band 1: (m,n) = (0,0)

$$E_{00}(\kappa) = E_0[1^2 + \kappa^2] = E_0(1 + \kappa^2)$$

Band 2: (m,n) = (-1,0)

$$E_{-1,0}(\kappa) = E_0[(-1)^2 + \kappa^2] = E_0(1 + \kappa^2)$$(degenerate with Band 1)

Band 3: (m,n) = (0,-1)

$$E_{0,-1}(\kappa) = E_0[1^2 + (\kappa - 2)^2] = E_0[1 + (\kappa - 2)^2]$$

Band 4: (m,n) = (-1,-1)

$$E_{-1,-1}(\kappa) = E_0[(-1)^2 + (\kappa - 2)^2] = E_0[1 + (\kappa - 2)^2]$$(degenerate with Band 3)

Band 5: (m,n) = (1,0)

$$E_{1,0}(\kappa) = E_0[3^2 + \kappa^2] = E_0(9 + \kappa^2)$$

6.6 Band Values at Key Points

At X point (κ = 0):

- Bands 1,2: $E = E_0(1 + 0) = E_0$
- Bands 3,4: $E = E_0[1 + (0 - 2)^2] = E_0(1 + 4) = 5E_0$
- Band 5: $E = E_0(9 + 0) = 9E_0$

At M point (κ = 1):

- Bands 1,2: $E = E_0(1 + 1) = 2E_0$
- Bands 3,4: $E = E_0[1 + (1 - 2)^2] = E_0(1 + 1) = 2E_0$
- Band 5: $E = E_0(9 + 1) = 10E_0$

6.7 Band Crossing Analysis

Bands cross when $E_{mn}(\kappa) = E_{m'n'}(\kappa)$

Example: Bands 1 and 3 cross when:

$$1 + \kappa^2 = 1 + (\kappa - 2)^2 \Rightarrow \kappa^2 = \kappa^2 - 4\kappa + 4 \Rightarrow 4\kappa = 4 \Rightarrow \kappa = 1$$

At κ = 1 (M point): $E = 2E_0$ for both bands.

6.8 Group Velocity and Effective Mass

Group velocity: $\mathbf{v}_g = \frac{1}{\hbar}\nabla_{\mathbf{k}}E(\mathbf{k})$

For Band 1: $E = E_0(1 + \kappa^2)$, with $k_y = \frac{\pi}{a}\kappa$

$$v_{g,y} = \frac{1}{\hbar}\frac{\partial E}{\partial k_y} = \frac{1}{\hbar}\frac{\partial E}{\partial \kappa}\frac{\partial \kappa}{\partial k_y} = \frac{1}{\hbar}(2E_0\kappa)(\frac{a}{\pi})$$

But $E_0 = \frac{\hbar^2}{2m}(\frac{\pi}{a})^2$, so:

$$v_{g,y} = \frac{1}{\hbar}(2 \cdot \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 \cdot \kappa)(\frac{a}{\pi}) = \frac{\hbar\pi}{ma}\kappa$$

Effective mass: $m^* = \hbar^2(\frac{\partial^2 E}{\partial k^2})^{-1}$

For Band 1: $\frac{\partial^2 E}{\partial k_y^2} = 2E_0(\frac{a}{\pi})^2 = \frac{\hbar^2}{m}$

Thus: $m^* = m$ (free electron mass)