Kronig–Penney model

Task 1

Given:

- $a = 1.5$ Å (well width)
- $b = 1.0$ Å (barrier width)
- $V(x)$ varies from 0 to 10 eV.

Model: Kronig–Penney model (delta-function limit when $b \to 0$ but here b fixed, finite rectangular barriers).

The band gap width between 1st and 2nd bands depends on the strength of the periodic potential.

Approximate gap formula (for delta-potential version):

$$V_0 b = P(\text{strength}), E_g \approx 2 \mid V_G \mid$$

where V_G is the Fourier component of potential for reciprocal vector $G = 2\pi/(a+b)$.

For finite rectangular barriers, the gap at $k = \pi/(a+b)$ (BZ boundary) increases with V_0.

Trend:

- When $V_0 = 0$, free electron → no gap.
- As V_0 increases, gap increases monotonically, saturating slowly.

Rough plot description:

- x-axis: V_0 (eV)
- y-axis: Band gap E_g (eV)
- Curve: Starts at (0,0), rises sharply for small V_0, then increases more slowly toward saturation.

$E_g(V_0) \propto$ something like$2\sqrt{V_0 E_1}$initially, then linear? Actually from KP equation:

KP equation:

$$\cos(ka) = \cos(k_1 a) + P\frac{\sin(k_1 a)}{k_1 a}, P = \frac{mV_0 ba}{\hbar^2} \quad \text{(in some units)}$$

Gap occurs when | RHS |> 1 is not possible → gap width $\Delta \approx 2V_0 \frac{\sin(\pi a/(a+b))}{\pi}$ for small V_0? Actually, known:

For delta-barrier: $E_g \approx 2V_0 b/a$ for small P, but here b fixed, so $E_g \propto V_0$ initially.

Conclusion for plot: Linear rise for small V_0, then sublinear, saturating.

Task 2

Given:

- $a = 1.5$ Å
- $V_0 = 5$ eV
- Vary barrier width b.

Effect: Increasing b increases the "duty cycle" of the barrier, increasing the effective potential strength.
In delta limit ($b \to 0$), $P = mV_0 ba/\hbar^2 \to$ gap proportional to $P \to$ proportional to b.
For finite b, the Fourier component V_G is:

$$V_G = \frac{1}{a+b}\int_0^b V_0 e^{-iGx} dx, G = 2\pi/(a+b)$$

$$| V_G | = \frac{V_0}{a+b} \left| \frac{1-e^{-iGb}}{iG} \right| = \frac{V_0}{a+b} \cdot \frac{2 | \sin(Gb/2) |}{G}$$

So $E_g \propto | V_G | \propto \frac{\sin(\pi b/(a+b))}{\pi/(a+b)}$.
Thus $E_g(b)$ increases from $b = 0$ to a maximum at $b/(a+b) = 0.5$ (when $\sin(\pi b/(a+b)) = 1$), then decreases to 0 when $b = a + b$ (all barrier, no well → no gap? Actually period changes). But physically, when b increases too much, the bands become flat, but gap max at $b \approx a$.
Rough plot:

- x-axis: b (Å) from 0 to ~3 Å
- y-axis: E_g
- Curve: Starts at 0 for $b = 0$, peaks around $b \approx a = 1.5$ Å, then decreases toward 0 as $b \to \infty$ (infinite barrier → isolated wells → degenerate levels → gap between bands? Actually gap between ground and first excited state in a well remains, but in periodic model, when b large, tunneling negligible, band width ~0, gap ~ fixed? Need care.)

Actually in KP model, as b increases with a fixed, potential becomes more like a square well array: gap between bands approaches the difference between quantized levels in a single well of width a. So gap saturates, not goes to 0. My earlier sine-form wrong for large b.
Better: For large b, $E_g \to E_2 - E_1$ of a well of size a, independent of b. So plot: increase, then saturate.

Task 3
Amorphous solid lacks long-range order but has short-range order (similar atomic spacing).
From Tasks 1 and 2:

- Gap depends on **potential strength** (related to atomic potential — chemical composition) and **spatial width of potential barrier/well** (related to atomic spacing and atomic size).

In amorphous solid:

- **Well depth** $V_0 \to$ determined by atomic nuclear charge and screening → chemical element.
- **Well width** $a \to$ related to nearest-neighbor distance (short-range order).

Thus, even without periodicity, if the short-range potential is similar to crystalline case (same atom type and bond length), the band gap can persist because the gap originates from the strong potential scattering at $k \approx \pi/$interatomic spacing, which exists in amorphous phase due to retention of short-range order.

Conclusion: Key short-range properties:

1. Atomic potential strength (atomic number)
2. Nearest-neighbor distance (well width)
3. Coordination (affects potential shape)

Example: SiO_2 amorphous: Si–O bond length and strong ionic potential → large gap ~9 eV.

Task 4

Bragg law: $2d\sin\,\theta = n\lambda$.

For electrons in crystal: $\lambda = 2\pi/k$, Bragg condition → $k = n\pi/d$.

At BZ boundary $k = \pi/d$, electrons satisfy Bragg condition → strong reflection → standing waves → band gap.

Electrons with k far from BZ boundary propagate freely (no Bragg reflection).

Crystal effect for other k:

- For k not near BZ boundary, nearly free electron behavior.
- Crystal potential causes **band curvature** (effective mass changes) due to $E(k)$ deviation from parabola.
- Also, for k near BZ center, small periodic perturbation → slightly lowered energy compared to free electron.

Task 5

Empty lattice model: $V = 0$, but impose periodicity — fold free electron dispersion into reduced zone scheme.

1D lattice period a.

Free electron: $E(k) = \frac{\hbar^2 k^2}{2m}$.

Reduced zone scheme: For any k in first BZ $(-\pi/a, \pi/a]$,

$$E_n(k) = \frac{\hbar^2}{2m}(k + \frac{2\pi n}{a})^2, n = 0, \pm1, \pm2, \ldots$$

First three bands ($n = 0, \pm1$):

- $n = 0$: $E_0(k) = \frac{\hbar^2 k^2}{2m}$ — parabola centered at $k = 0$.
- $n = -1$: $E_{-1}(k) = \frac{\hbar^2}{2m}(k - \frac{2\pi}{a})^2$ — in 1BZ, shift equivalent to $k + 2\pi/a$ → actually $k - 2\pi/a$ mapped to k in 1BZ: Let $k' = k - 2\pi/a$, in 1BZ k' is $k - 2\pi/a$ if $k > 0$ small? Better:
  Actually $n = -1$: $k - 2\pi/a$ → in reduced zone, use $k - 2\pi/a = k - G$ with $G = 2\pi/a$, so $E(k) = \frac{\hbar^2}{2m}(k - 2\pi/a)^2$, but for k in 1BZ, plot that.

Better: Explicit:

Let $G = 2\pi/a$.

Band 1 ($n = 0$): $E = \frac{\hbar^2 k^2}{2m}$, minimum 0 at $k = 0$.

Band 2 ($n=-1$): $E=\frac{\hbar^2(k-G)^2}{2m}$. In 1BZ, at $k=-\pi/a$, $k-G=-\pi/a-2\pi/a=-3\pi/a$, $E=\frac{\hbar^2(9\pi^2/a^2)}{2m}$. At $k=\pi/a$, $k-G=\pi/a-2\pi/a=-\pi/a$, $E=\frac{\hbar^2\pi^2/a^2}{2m}$. So it's a parabola decreasing from $k=-\pi/a$ to $k=\pi/a$.

Band 3 ($n=1$): $E=\frac{\hbar^2(k+G)^2}{2m}$. At $k=-\pi/a$, $k+G=\pi/a$, $E=\frac{\hbar^2\pi^2/a^2}{2m}$. At $k=\pi/a$, $k+G=3\pi/a$, $E=\frac{\hbar^2 9\pi^2/a^2}{2m}$, so increasing parabola.

Wavefunction:

$$\psi_{nk}(x)=e^{ikx}u_{nk}(x), u_{nk}(x)=\text{const}\cdot e^{iG_nx}, G_n=n\frac{2\pi}{a}.$$

So $\psi_{nk}(x)\propto e^{i(k+G_n)x}$ — plane wave.

Plot: In 1BZ, three bands:

- n=0: upward parabola from 0 at k=0 to $\hbar^2(\pi/a)^2/2m$ at edges.
- n=-1: symmetric with n=1 actually degenerate at BZ boundary. Actually at $k=\pi/a$, n=-1 and n=1 both have $E=\hbar^2(\pi/a)^2/2m$. At $k=0$, n=-1: $E=\hbar^2(2\pi/a)^2/2m$, n=1 same. So band 2 and 3 are degenerate at center and boundaries? Wait, check:

At $k=0$:
n=-1: $E=(-2\pi/a)^2=4\pi^2/a^2$ times $\hbar^2/2m$
n=1: same.
So bands 2 and 3 are degenerate everywhere? No, because at k nonzero, (k+G) and (k-G) magnitudes differ unless k=0. Actually they're degenerate only at k=0.
So bands:
Band 1: bottom 0 at k=0
Band 2 & 3: both start at $4\pi^2\hbar^2/2ma^2$ at k=0, then one decreases to $\pi^2\hbar^2/2ma^2$ at k=π/a (n=-1), the other increases to $9\pi^2\hbar^2/2ma^2$ at k=π/a (n=1). So they cross.
In empty lattice, no gap at crossing.

Task 6

2D square lattice, lattice constant a.

Reciprocal lattice vectors: $\mathbf{G}=(m,n)\frac{2\pi}{a}$.

Path X to M:
X point: $(\pi/a,0)$
M point: $(\pi/a,\pi/a)$
So we vary k_y from 0 to π/a, keeping $k_x=\pi/a$.

Empty lattice bands:

$$E(\mathbf{k})=\frac{\hbar^2}{2m}|\mathbf{k}+\mathbf{G}|^2$$

with $\mathbf{k}=(\pi/a,k_y)$.

Choose small $\mathbf{G}$ values:
$\mathbf{G}=(0,0),(\pm1,0),(0,\pm1),(\pm1,\pm1),(-1,1),(1,-1)$ etc.

Compute for each:

1. $G = (0,0)$:
$$\mathbf{k} + \mathbf{G} = (\pi/a, k_y)$$
$E = \frac{\hbar^2}{2m}[(\pi/a)^2 + k_y^2]$ — increases with k_y.
2. $G = (-1,0) \cdot 2\pi/a = (-2\pi/a, 0)$:
$$\mathbf{k} + \mathbf{G} = (\pi/a - 2\pi/a, k_y) = (-\pi/a, k_y)$$
Same magnitude as above → degenerate with G=(0,0) band.
3. $G = (0,-1) \cdot 2\pi/a = (0, -2\pi/a)$:
$$\mathbf{k} + \mathbf{G} = (\pi/a, k_y - 2\pi/a)$$
Magnitude: $(\pi/a)^2 + (k_y - 2\pi/a)^2$ — large at $k_y = 0$, min at $k_y = 2\pi/a$ outside range.
4. $G = (-1,-1) \cdot 2\pi/a = (-2\pi/a, -2\pi/a)$:
$\mathbf{k} + \mathbf{G} = (-\pi/a, k_y - 2\pi/a)$ magnitude same as above case symmetric.

Better to list few lowest at $k_y = 0$ (X point):

At X: $k_x = \pi/a, k_y = 0$:

- G=(0,0): $E = (\pi/a)^2$ in units $\hbar^2/2m$.
- G=(-1,0): same as above.
- G=(0,-1): $(\pi/a)^2 + (2\pi/a)^2 = 5(\pi/a)^2$
- G=(-1,-1): same 5.
- G=(1,0): $(3\pi/a)^2 = 9$
- G=(0,1): $(\pi/a)^2 + (2\pi/a)^2 = 5$ again.

So lowest band: doubly degenerate E=1 unit at X.

As k_y increases, these bands disperse.

We can plot E vs k_y from 0 to π/a for these G's.

Bands:

Band1: G=(0,0) & (-1,0) degenerate: $E = 1 + k_y^2$ in units of $(\pi/a)^2\hbar^2/2m$.

Band2: G=(0,-1) & (-1,-1): $E = 1 + (k_y - 2)^2$ but 2 in units of π/a, so at $k_y = 0$, E=1+4=5, at $k_y = 1$, E=1+1=2, at $k_y = 1$ (M point), E=2.

Band3: G=(1,0): $E = (3)^2 + k_y^2 = 9 + k_y^2$ — high.

Band4: G=(0,1): $E = 1 + (k_y + 2)^2$ at $k_y = 0$, E=5, increases.

Band5: G=(1,1): $E = (3)^2 + (k_y + 2)^2$ very high.

So five lowest bands: two low ones (degenerate), then next at E=5 at X, splitting with k_y.

Plot: E vs k_y from 0 to 1 (in units of π/a), energies in units of $(\pi^2\hbar^2)/(2ma^2)$.