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EE 381: Electronic Properties of Materials
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**Homework 1**

## 1. Free electron: relation between $E$ and $k$

**Classical → de Broglie.** For a free electron ($V = 0$) the classical kinetic energy is

$$E = \frac{p^2}{2m}.$$

De Broglie gives $p = h/\lambda = \hbar k$ (with $k = 2\pi/\lambda$). Hence

$$\boxed{E = \frac{\hbar^2 k^2}{2m}}.$$

**Schrödinger derivation.** The time-dependent Schrödinger equation with $V = 0$ is

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi.$$

Insert a plane wave $\psi(\mathbf{r}, t) = e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$:

$$i\hbar(-i\omega)\psi = \frac{\hbar^2}{2m}(k^2)\psi \quad \Rightarrow \quad \hbar\omega = \frac{\hbar^2 k^2}{2m}.$$

Identifying $E = \hbar\omega$ gives the same dispersion,

$$\boxed{E = \frac{\hbar^2 k^2}{2m}}.$$

## 2. Kronig–Penney square-wave potential (period $P = 5\,\text{nm}$)

**Setup.** One period consists of a *well* of width $a = 4\,\text{nm}$ with $U = 0$ and a barrier of width $b = 1\,\text{nm}$ with $U_0 = 1\,\text{eV}$. Let $m = m_e$. For a piecewise-constant periodic potential, Bloch's theorem yields the Kronig–Penney dispersion

$$\cos(k_B P) = \begin{cases} \cos(k_1 a)\cosh(\kappa b) - \dfrac{k_1^2 - \kappa^2}{2k_1\kappa}\sin(k_1 a)\sinh(\kappa b), & E < U_0, \\ \cos(k_1 a)\cos(k_2 b) - \dfrac{k_1^2 + k_2^2}{2k_1 k_2}\sin(k_1 a)\sin(k_2 b), & E > U_0, \end{cases}$$

with

$$k_1 = \frac{\sqrt{2mE}}{\hbar}, \qquad \kappa = \frac{\sqrt{2m(U_0 - E)}}{\hbar}, \qquad k_2 = \frac{\sqrt{2m(E - U_0)}}{\hbar}.$$

**Allowed energies** (bands) satisfy $\boxed{|\cos(k_B P)| \le 1}$; otherwise the energy is forbidden (gap).

**Can an electron with $E > U_0$ take any energy?** No. Even for $E > U_0$ both regions are propagating, but the periodic modulation produces Bragg scattering and band gaps. Thus *some* energies above $1\,\text{eV}$ are still forbidden: only those giving $|\cos(k_B P)| \le 1$ are allowed.

**Numerical check at $E = 1.05\,\mathbf{eV}$.** Constants used: $\hbar = 1.0545718 \times 10^{-34}$ J s, $m_e = 9.1093836 \times 10^{-31}$ kg, $1\,\text{eV} = 1.6021766 \times 10^{-19}$ J.

For $E = 1.05\,\text{eV}$ ($> U_0$):

$$k_1 = \frac{\sqrt{2m_e E}}{\hbar} \;\approx\; 5.2497 \times 10^9\ \text{m}^{-1}, \qquad k_1 a \approx 20.999,$$

$$k_2 = \frac{\sqrt{2m_e(E - U_0)}}{\hbar} \;\approx\; 1.1456 \times 10^9\ \text{m}^{-1}, \quad k_2 b \approx 1.1456.$$

Plugging these into the $E > U_0$ formula,

$$\cos(k_B P) = \cos(k_1 a)\cos(k_2 b) - \frac{k_1^2 + k_2^2}{2k_1 k_2}\sin(k_1 a)\sin(k_2 b) \;\approx\; -2.056.$$

Since $|\cos(k_B P)| \approx 2.056 > 1$, $E = 1.05\,\mathbf{eV}$ **is forbidden** (lies in a band gap).

**First few Band Ranges.** Evaluating $|\cos(k_B P)| \le 1$ over energy shows alternating allowed/forbidden intervals. For this geometry, the first several allowed bands (rounded) are

0.01946–0.01954 eV, 0.07766–0.07804 eV, 0.17406–0.17512 eV,

0.30755–0.31008 eV, 0.47587–0.48175 eV, 0.67405–0.68826 eV,

0.88954–0.92658 eV, 1.09322–1.19190 eV, 1.26333–1.44557 eV, 1.47701–1.69817 eV, …