Numerical

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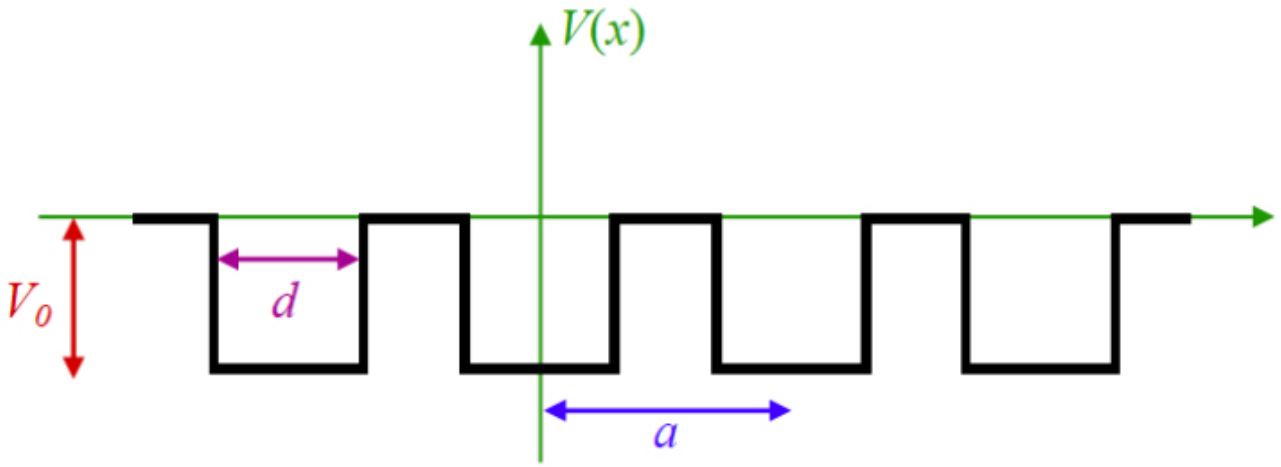
Consider a 1D Kronig-Penney model with lattice parameter a and potential wells with depth V_0 and size d, as shown in the graph:



The periodic potential V(x) in the region of $-a/2 < x < a/2$ is written as

$$V_x = \begin{cases} -V_0, \ -d/2 < x < d/2. \\ 0, \ -a/2 < x < d/2 \text{ or } d/2 < x < a/2. \end{cases} \tag{1}$$

Solve the Schrodinger equation using plane wave basis set:

$$u_{n,k} = \sum_{l'=-N}^{N} c_{l'}^{(nk)} \frac{1}{\sqrt{a}} e^{ix\frac{2\pi l'}{a}} \tag{2}$$

For each k, the Hamiltonian , $H_k = T_k + V(x)$, where $T_k = \frac{\hbar^2}{2m_e}(\frac{1}{i}\frac{d}{dx} + k)^2$. Using the plane wave basis set. Write down the analytical forms of matrices $[T_k]_{l,l'}$ and $[V]_{l,l'}$.

Ans. The Schrodinger equation using the Bloch theorem:

$$\psi_{n,k}(x) = e^{ikx} u_{n,k}(x)$$

where the periodic function $u_{n,k}(x)$ is expanded in a plane wave basis:

$$u_{n,k}(x) = \sum_{l'=-N}^{N} c_{l'}^{(n,k)} \frac{1}{\sqrt{a}} e^{i\frac{2\pi l'}{a}x}$$

The full Hamiltonian for a given k is:

$$H_k = T_k + V(x)$$

where

$$T_k = \frac{\hbar^2}{2m_e}\left(-i\frac{d}{dx} + k\right)^2$$

The matrix elements of T_k and $V(x)$ in the plane wave basis:

$$\phi_l(x) = \frac{1}{\sqrt{a}} e^{i\frac{2\pi l}{a}x}$$

Kinetic Energy Matrix:

Applying the kinetic operator to the basis:

$$T_k \phi_{l'}(x) = \frac{\hbar^2}{2m_e} \left(\frac{2\pi l'}{a} + k \right)^2 \phi_{l'}(x)$$

The plane waves are orthonormal, the matrix is diagonal:

$$[T_k]_{l,l'} = \langle \phi_l | T_k | \phi_{l'} \rangle = \delta_{l,l'} \cdot \frac{\hbar^2}{2m_e} \left(\frac{2\pi l}{a} + k \right)^2$$

Potential Energy Matrix:

We compute the matrix elements of the potential:

$$[V]_{l,l'} = \langle \phi_l | V(x) | \phi_{l'} \rangle = \frac{1}{a} \int_{-a/2}^{a/2} V(x) e^{-i\frac{2\pi l}{a}x} e^{i\frac{2\pi l'}{a}x} dx = \frac{1}{a} \int_{-d/2}^{d/2} (-V_0) e^{i\frac{2\pi (l'-l)}{a}x} dx$$

Let $\Delta l = l' - l$:

- If $\Delta l = 0$:

$$[V]_{l,l} = -\frac{V_0}{a} \int_{-d/2}^{d/2} dx = -\frac{V_0 d}{a}$$

- If $\Delta l \neq 0$:

$$[V]_{l,l'} = -\frac{V_0}{a} \int_{-d/2}^{d/2} e^{i\frac{2\pi \Delta l}{a}x} dx = -\frac{V_0}{a} \cdot \frac{2\sin\left(\pi \Delta l \frac{d}{a}\right)}{\frac{2\pi \Delta l}{a}} = -V_0 \cdot \frac{\sin\left(\pi \Delta l \frac{d}{a}\right)}{\pi \Delta l}$$

Final Matrix Forms:

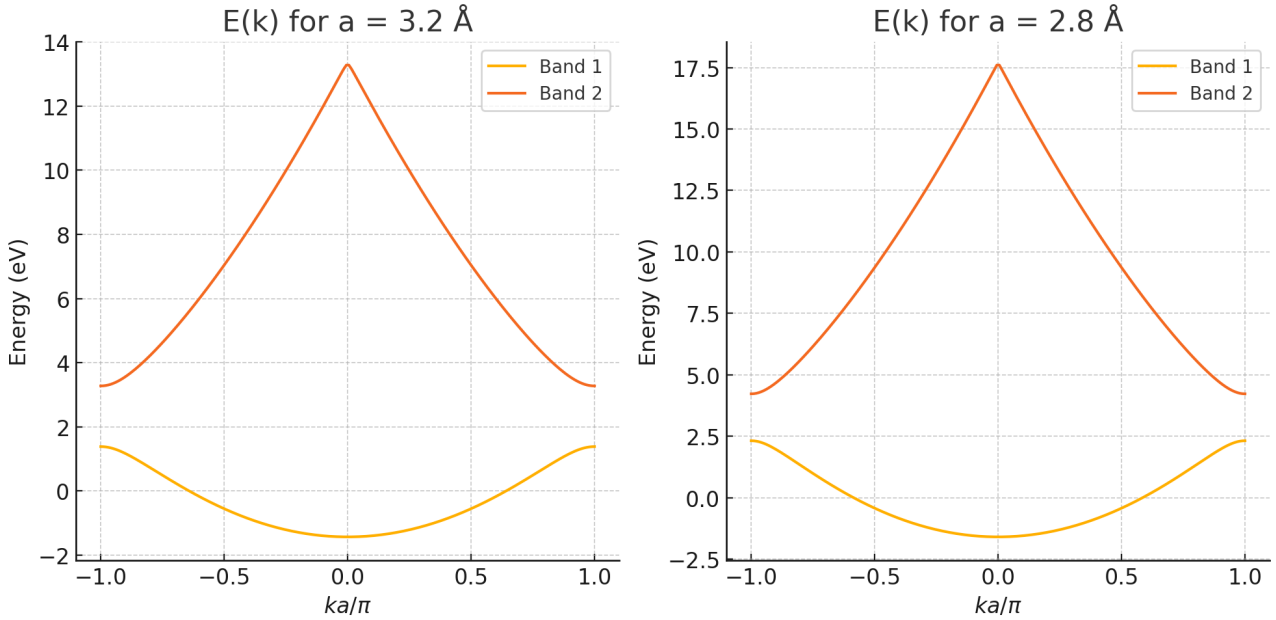
Kinetic Energy:

$$[T_k]_{l,l'} = \delta_{l,l'} \cdot \frac{\hbar^2}{2m_e} \left(\frac{2\pi l}{a} + k \right)^2$$

Potential Energy:

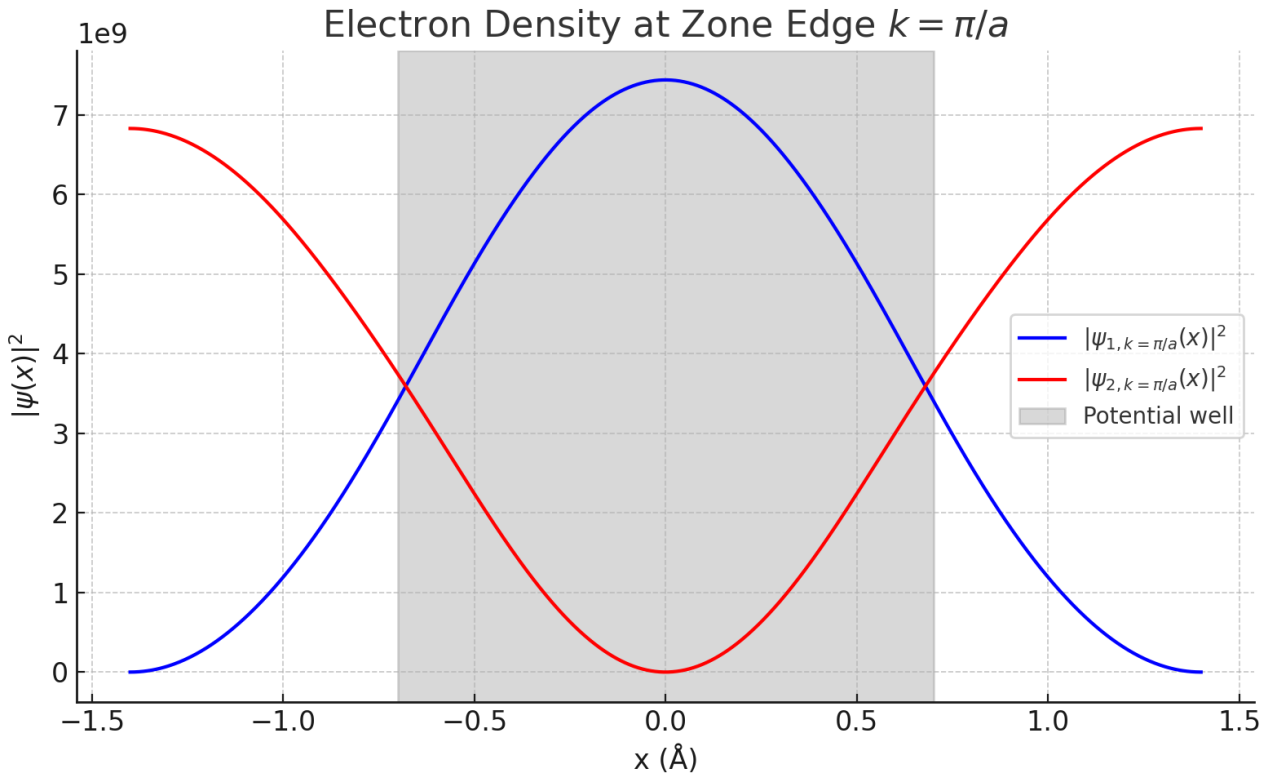
$$[V]_{l,l'} = \begin{cases} -\dfrac{V_0 d}{a}, & l = l' \\ -\dfrac{V_0 \sin\left(\pi (l'-l) \dfrac{d}{a}\right)}{\pi (l'-l)}, & l \neq l' \end{cases}$$

b. Consider, a = 3.2 Å, $V_0 = 3.0$ eV, and d = 1.4 Å. Plot the energy dispersion E(k) of the lowest two bands. Find out the band width W and the energy minimum E_0 of the lowest band, and the band gap E_g. Determine, what is the value of N would give you convergent results. Compare results when, a = 2.8 Å, $V_0 = 3.0$ eV, and d = 1.4 Å. Plot the energy dispersion E(k) of the lowest two bands. Find out the band width W and the energy minimum E_0 of the lowest band, and the band gap E_g. Determine, what is the value of N would give you convergent results. How does the band width (W) vary with the lattice parameter (a)? Explain why.
Ans. For $a = 3.2$ Å:
Minimum Energy of Lowest Band (E_0): 0.0303 eV, bandwidth (W): 0.1464 eV, and band gap (E_g): 0.2152 eV.
For $a = 2.8$ Å:
Minimum Energy of Lowest Band (E_0): 0.0613 eV, bandwidth (W): 0.2596 eV, and band gap (E_g): 0.2561 eV.
Convergence is at N $\geq$ 7, so N = 7 gives reliable convergence. Relation between bandWidth (W) and lattice parameter (a): When lattice constant, a decreases, the bandwidth, W increases. This is because, a smaller a means the potential wells are closer together. This increases the overlap of electron wavefunctions between adjacent wells. Stronger overlap will result in higher tunneling probability and wider energy bands.



c. Plot the electron density $|\psi_{n,k}(x)|^2$ of the lowest two states at the zone edge ($k = \pi/a$). Discuss how the electron density of these two states relate to their energy.
Ans. Band 1 given in blue curve shows the ground State at $k = \pi/a$ The electron density is maximal inside the potential well (gray shaded region). This indicates that the electron prefers to localize in the attractive region (i.e., the potential well where $V(x) = -V_0$. As a result, this state has lower kinetic and potential energy, making it the ground state.

While, band 2 (Red Curve) – First Excited State at $k = \pi/a$. The electron density is minimized in the well, with peaks appearing outside the potential well. This corresponds to an anti-bonding-like state, where the wavefunction changes sign and has nodes near the well. Because the electron avoids the attractive well region, this leads to higher energy.



Energy difference between the two states arises from their spatial distribution. The ground state constructively interferes within the well (lower energy). The excited state destructively interferes near the well (higher energy).

This behavior at $k = \pi/a$ is a related to of Brillouin zone edge states where band splitting originates due to Bragg reflection and periodic potential.