

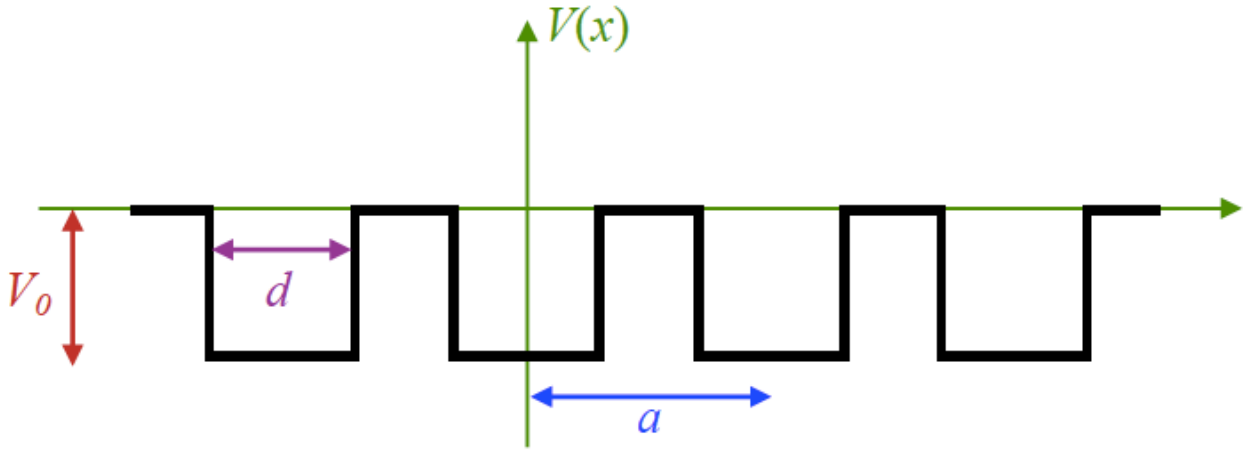
1D Kronig-Penney model

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

$$V(x) = \begin{cases} -V_0, & -d/2 < x < d/2 \\ 0, & -a/2 < x < d/2 \quad \text{or} \quad d/2 < x < a/2. \end{cases}$$

Here we solve the Schrödinger equation using the plane-wave basis set:

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



- (a) For each k , the Hamiltonian $H_k = T_k + V(x)$, where $T_k = \frac{\hbar^2}{2m_e} \left(\frac{1}{i} \frac{d}{dx} + k \right)^2$. Using the plane wave basis set, write down the analytical forms of matrices $[T_k]_{l,l'}$ and $[V]_{l,l'}$.
- (b) Consider $a = 2.8 \text{ \AA}$, $V_0 = 3.0 \text{ eV}$, and $d = 1.4 \text{ \AA}$. Plot the energy dispersion $E_n(k)$ 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 . Notice that the first thing you need to do is to determine what N would give you convergent results.
- (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.
- (d) Consider $a = 3.2 \text{ \AA}$, $V_0 = 3.0 \text{ eV}$, and $d = 1.4 \text{ \AA}$. Plot the energy dispersion $E_n(k)$ 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 . Again, you need to determine an appropriate N first. Compare your results in (b) and (d), how does the band width (W) vary with the lattice parameter (a)? Explain why.