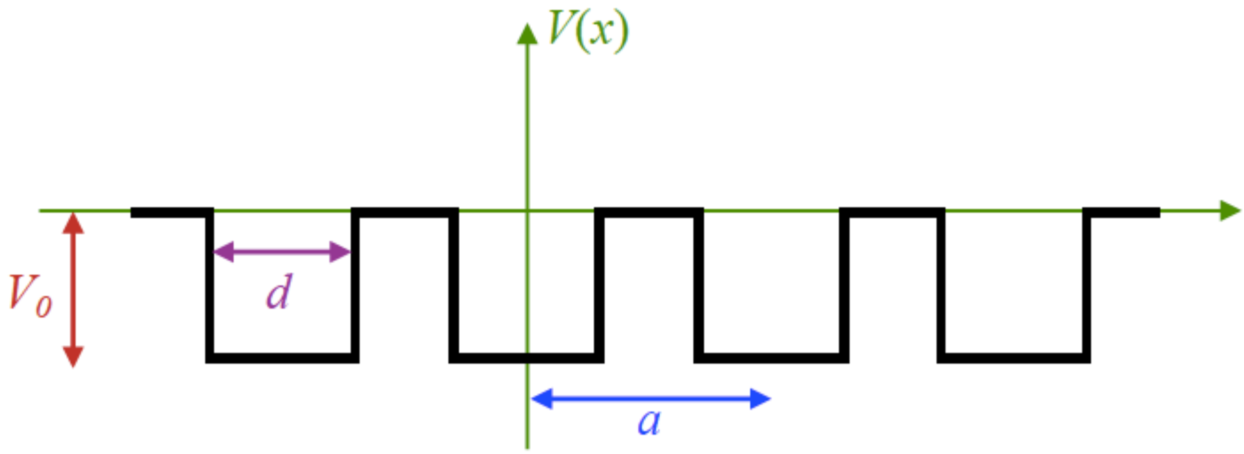
1D Kronig-Penney model

Consider a 1D Kronig-Penney model with lattice parameter a and potential wells with depth $V0$ 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 Å, V_0 = 3.0 eV, and d = 1.4 Å. 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 Å, V_0 = 3.0 eV, and d = 1.4 Å. Plot the energy dispersion $En(k)$ 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.