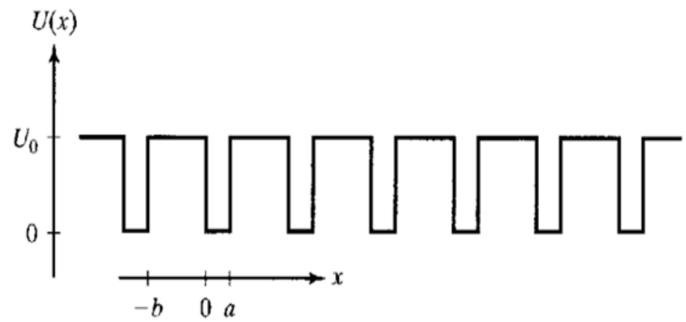
MATLAB Assignment:

1. Solve the time independent 1D Schrodinger's equation numerically for the potential $U=3x+7x^4+x^2+2$ and obtain the Eigen values of energies for first 100 level.
2. The Kronig-Penney model and solution of it, obtained using continuity conditions and Bloch's theorem, is shown below. Equation 1 relates the E and indices k of possible Bloch functions. This equation has real solutions for k in certain energy intervals, for $|\cos(k(a+b))|<1$. These solutions correspond to wavelike solutions. For $|\cos(k(a+b))|>1$, there are no Bloch electrons and corresponding energy intervals are denoted as band gaps. You need to implement equation 1 and investigate several physical situations. For all the calculations use $m_o$=9.1e-31 kg, $\hbar$= 6.58199e-16 eV.s/rad.




$$-\frac{\alpha^2+\beta^2}{2\alpha\beta}\sin\alpha a \sin\beta b + \cos\alpha a \cos\beta b = \cos k(a+b) \qquad \textbf{(1)}$$

**Where**

$$\alpha = \sqrt{2mE/\hbar^2}$$

$$\beta = \begin{cases} i\beta_-; & \beta_- = \sqrt{2m(U_0 - E)/\hbar^2} \quad 0 < E < U_0 \\ \beta_+; & \beta_+ = \sqrt{2m(E-U_0)/\hbar^2} \quad E > U_0 \end{cases}$$

(a) Using equation 1, plot the E-K relation for free electron.

(b) Take different values of $U_o$ (= 0.1, 0.2, and 0.5 eV) and solve equation 1 for nearly free electron considering $E=U_o/2$ and $E= 1.01*U_o$. Assume a=0.25*b=1Å. Plot dispersion relation and wave function for first 10 period. Are the wave function in the adjacent wells are interacting with each other.

(c) Consider $U_o$=5 eV and a=0.25*b=1Å. Find the band structure for strong potential. Comment on the shape of allowed solutions and dispersion relation. Plot the wave function for first 10 period. Are the wave function in the adjacent wells are interacting with each other.

(d) Consider the free atom limit ($U_o$=1000eV) such that barrier between the adjacent wells is effectively infinite. Plot the dispersion relation.