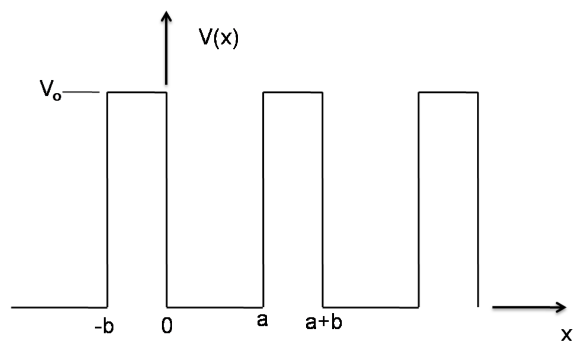
1. The Kroenig-Penny model uses a simple "square well" periodic potential for an electron in a 1-D solid of length L. This potential is shown below, where V_o is the height of the barrier (measured in eV).



(a) We will look for solutions to Schrödinger's equation which are Bloch functions of the form $\Psi(x) = U(x)e^{ikx}$. In this solution, k is still quantized ($k = n\pi/L$, $n = 0, \pm1, \pm2,...$). Use this solution in the time-independent Schrödinger equation to find a set of four simultaneous equations. Show that the four equations reduce to the following equation:

$$\frac{\beta^2 - \alpha^2}{2\alpha\beta} \sin(\alpha a) \sinh(\beta b) + \cos(\alpha a) \cosh(\beta b) = \cos[k(a + b)], \quad (1)$$

where $\alpha = \frac{\sqrt{2mE}}{\hbar}$ and $\beta = \frac{\sqrt{2m(V_o - E)}}{\hbar}$. This is the relationship between E and k in the Kroenig-Penny model.

(b) For the free electron model, with quantized values of k, write down the relationship between E and k. (This should take you all of three seconds).

(c) Assume L=42Å. For the free electron model, calculate the first 45 non-zero energy levels in eV.

(d) Now we return to the Kroenig-Penny model. Assume $a = 2.00$Å, $b = 0.10$Å, $V_o = 200$ eV, and $L = 20(a + b)$. In the Kroenig-Penny model, we want to calculate the first 45 non-zero energy levels (in eV).

Since E appears in 8 different places on the left-hand side of Eq. 1, it would be very difficult to calculate an energy value using a known k value. But it is easy to go from a known E value to calculate a corresponding k value. We can pick some reasonable values for E, from each of which we can calculate a value for k using Eq. 1. This calculated value for k may not be an allowed one, but we can use interpolation to find a new energy value that would be an allowed value of k.

Note that some energy levels may be higher than 200 eV, which means β will become imaginary. Eq. 1 is still valid and can be used after re-writing it using $\cosh(ix) = \cos(x)$ and $\sinh(ix) = i \sin(x)$.

i. To help you find reasonable values of E, try two things. First, remember the E values you calculated for the free electron model. Second, plot the left-hand-side (LHS) of Eq. 1 as a function of energy up to 400 eV. What does it mean if $-1 < \text{LHS} < 1$? What does it mean if $\text{LHS} > 1$ or $\text{LHS} < -1$? You don't need to worry about when β becomes imaginary, MatLab will take care of that.

ii. Find the first 45 non-zero energy levels in eV for the Kroenig-Penny model. There are a number of ways to do this; I used `fzero`. Basically, `fzero` does the iteration method for you, although you can do it by hand. If you use `fzero`, be careful with how you pick your initial guesses! You can also do it by hand. However you decide to complete the problem, please give me your MatLab code.

(e) Plot E vs. k for the free electron model *and* the Kroenig-Penny model on the same graph. Discuss the results. Do you see energy bands in the Kroenig-Penny model? In the free electron model?