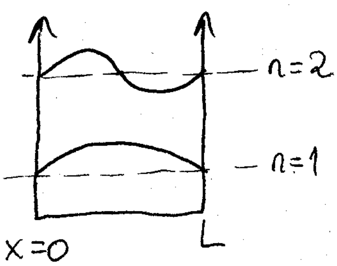
1. An infinite potential well for trapping electrons has walls at $x=0$ and $x=L$.
a. Solve the time-independent Schrodinger equation for this potential (you may leave the normalization as a variable). Be explicit about using boundary conditions.
b. Derive the formula for the permitted energies of particles in this box: $E_n = \frac{\hbar^2\pi^2 n^2}{2m_e L^2}$

The potential well contains 6 electrons: 2 each in the n=1 state, 2 in the n=2 state and 2 in the n=3 state.

c. Compute the total energy of the system (in eV) if the width of the box L=0.1nm.
d. How much energy (work) in eV is required to compress the system to 1/2 of its original size?

a)



(a) Outside well, $\psi = 0$

Inside well, $\frac{-\hbar^2}{2m_e}\frac{d^2\psi}{dx^2} = E\psi$ (*)

General solution: $\psi = a e^{ikx} + b e^{-ikx}$

where k is given by $E = \frac{\hbar^2 k^2}{2m_e}$ (subs. into (*))

Boundary conditions:

$\psi = 0$ at $x=0 \Rightarrow a + b = 0$, i.e. $b = -a$ so $\psi = a(e^{ikx} - e^{-ikx})$

(left→right wave + equal right→left wave)

$\psi = a(e^{ikx} - e^{-ikx}) = A\sin kx$ where $A = \frac{a}{2i}$

$\psi = 0$ at $x = L \Rightarrow A \sin kL = 0$. Only works if $kL = n\pi$; $n = 1, 2, 3$

b) From above $E = \frac{\hbar^2 k^2}{2m}$, so with allowed $k_n = \frac{n\pi}{L}$ $E_n = \frac{\hbar^2\pi^2 n^2}{2m_e L^2}$ as required

c) For six e^-, total energy $E_{tot} = \frac{2\hbar^2\pi^2}{2m_e L^2}(1^2+2^2+3^2) = \frac{14\hbar^2\pi^2}{m_e L^2}$

i.e. $E_{tot} = \frac{14}{4}\frac{(hc)^2}{m_e c^2 L^2} = \frac{14}{4}\frac{(1240\,eVnm)^2}{511\times10^3\times0.1^2} = \underline{1053.2eV}$

d) $E_n \propto \frac{1}{L^2}$ so $E_{tot} \propto \frac{1}{L^2}$ ∴ halving $L \Rightarrow E_{tot} \uparrow$ by factor 4.

$\Rightarrow$ new $E_{tot}(L/2) = 4E_{tot}(L)$ from part (c)

∴ Work done $= E_{tot}(L/2) - E_{tot}(L) = 3E_{tot}(L) = 3160eV$.

2. A particle of mass m is placed in a "half-infinite" potential well, which has potential energy $U \rightarrow \infty$ for $x<0$, $U=0$ for $0<x<a$, and $U=U_0$ for $x>a$. Here we consider three energy states, one at a time. When sketching the wavefunctions on top of the potential diagram, use the dashed line as the $\psi=0$ axis in each case.

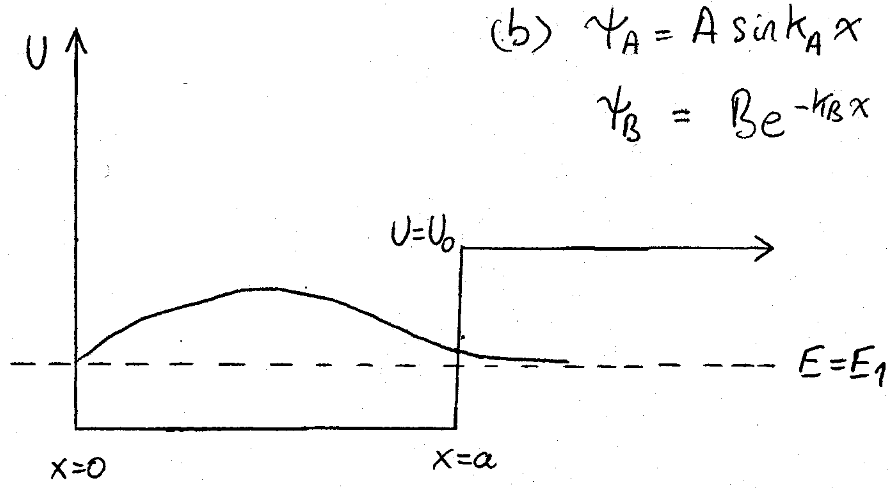
a. Sketch the wavefunction for first bound state ($n=1$) with $E_1<U_0$

b. Using the boundary condition $\psi=0$ at $x=0$, write down the functional form of the wavefunction: ψ_A for $x<a$, and ψ_B for $x>a$. (Use the normalization constants A for ψ_A and B for ψ_B - these constants are the maximum value of ψ in each region. You may also use the wavenumber k_A (for $x<a$), and "penetration depth" $1/k_B$ (for $x>b$) in each region to simplify your math, where each is defined according to: $E=\dfrac{\hbar^2 k_A^2}{2m}$; $(U_0-E)=\dfrac{\hbar^2 k_B^2}{2m}$).

c. Use the boundary conditions at $x=a$ to find a relation between ~~A and B in terms of~~ k_A and k_B (do not attempt to solve this equation - it can only be solved numerically to give an allowed value of the energy $E=E_1$).

d. Give an expression for the probability of detecting a particle in the "classically forbidden zone" $x>a$ in terms of B and k_B.

a)



(b) $\psi_A = A \sin k_A x$ since $\psi_A = 0$ at $x=0$

$\psi_B = Be^{-k_B x} + \cancel{Ce^{+k_B x}}$ $C=0$ otherwise $\psi \to \infty$.

c) At $x=a$: $\psi_A = \psi_B \Rightarrow \underline{A\sin(k_A a) = B}$ (1) $\dfrac{d\psi_A}{dx} = \dfrac{d\psi_B}{dx} \Rightarrow \underline{A k_A \cos(k_A a) = -k_B B}$ (2)

Divide (1) by (2) $\Rightarrow \dfrac{\tan(k_A a)}{k_A} = -\dfrac{1}{k_B}$ or $\tan(k_A a) = -\dfrac{k_A}{k_B}$ solve numerically for "allowed" $E_1, E_2, \ldots$

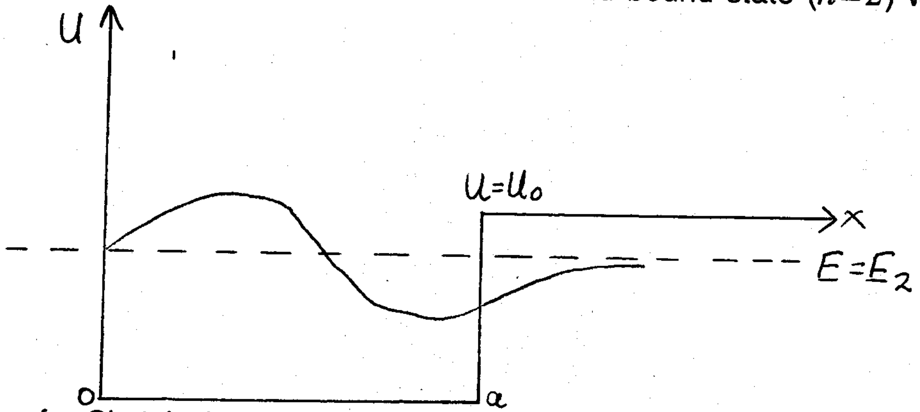
d) $\text{Prob}(x>a) = \displaystyle\int_{x=a}^{\infty} |\psi|^2 dx = |B|^2 \int_a^{\infty} e^{-2k_B x} = \frac{|B|^2}{2k_B}\left[e^{-2k_B a} - 0\right]$

$= \dfrac{|B|^2}{2k_B} e^{-2k_B a}$

Question 2 continued...

e. Sketch the wavefunction for the 2nd bound state ($n=2$) with energy $E_2<U_0$.

e)

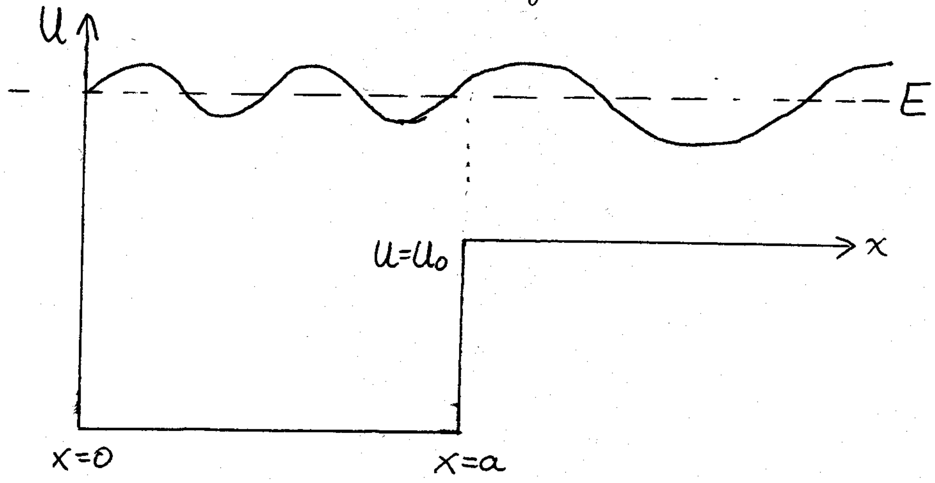


f. Sketch the wavefunction for an unbound state with total energy $E=2U_0$.

g. Write down the functional form of this state's wavefunction ψ_A for $x<a$ and ψ_B for $x>a$.

h. For this unbound state, what is the de Broglie wavelength of the particle for (i) $x<a$ and (ii) $x>a$, in terms of U_0?

f)



g) $x<a$: $\psi_A = A\sin k_A x$ as before

$x>a$: $\psi_B = B\sin(k_B x+\phi) = b_1 \sin k_B x + b_2 \cos k_B x = b_3 e^{ikx} + b_4 e^{-ikx}$

h) For $x<a$, $U=0$, $E=2U_0 \Rightarrow k_A = \dfrac{\sqrt{2m(E-U)}}{\hbar} = \sqrt{\dfrac{4mU_0}{\hbar^2}}$

$\Rightarrow \lambda_A = \dfrac{2\pi}{k_A} = \dfrac{2\pi\hbar}{\sqrt{4mU_0}} = \dfrac{h}{2\sqrt{mU_0}}$

For $x>a$, $U=U_0$, $E=2U_0 \Rightarrow k_B = \dfrac{\sqrt{2mU_0}}{\hbar} = \dfrac{k_A}{\sqrt{2}}$

$\Rightarrow \lambda_B = \dfrac{h}{\sqrt{2mU_0}} = \sqrt{2}\,\lambda_A$