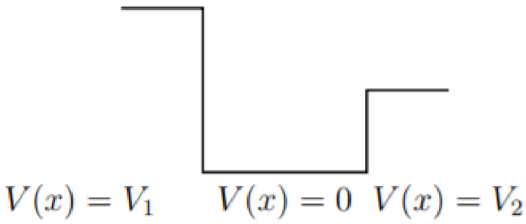
PH107 D1T5: Tutorial 8

12-02-2022

PARTICLE IN A FINITE BOX

Question 1

Consider the asymmetric finite potential well of width L, with a barrier V_1 on one side and a barrier V_2 on the other side. Obtain the energy quantization condition for the bound states in such a well. From this condition derive the energy quantization conditions for a semi-infinite potential well (when $V_1 \to \infty$ and V_2 is finite).



We are looking for a bound state, i.e. an energy eigenstate whose energy eigenvalue $E < V(\pm\infty) \implies E < V_2$ (WLOG we assume $V_2 < V_1$).
From TISE:

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} = \begin{cases} k_1^2 & x < 0 \\ -k^2 & 0 \le x \le L \\ k_2^2 & x > L \end{cases}$$

$$\psi(x) = \begin{cases} Ae^{k_1 x} + Be^{-k_1 x} & x < 0 \\ C\cos(kx) + D\sin(kx) & 0 \le x \le L \\ Ee^{k_2 x} + Fe^{-k_2 x} & x > L \end{cases}$$

Where

$$\begin{aligned} k_1^2 &= \frac{2m(V_1 - E)}{\hbar^2} \\ -k^2 &= \frac{-2mE}{\hbar^2} \\ k_2^2 &= \frac{2m(V_2 - E)}{\hbar^2} \end{aligned}$$

Since $\psi(x)$ cannot blow up at $\pm\infty, B = E = 0$
Continuity and Differentiability at $x = 0$

$$\begin{aligned} A &= C \\ Ak_1 &= Dk \end{aligned} \tag{1}$$

Continuity and Differentiability at $x = L$

$$\begin{aligned} C\cos(kL) + D\sin(kL) &= Fe^{-k_2 L} \\ -k(C\sin(kL) - D\cos(kL)) &= -k_2 F e^{-k_2 L} \end{aligned} \tag{2}$$

Put values of C and D from (1) and divide equations in (2)

$$\begin{aligned} \frac{\sin(kL) - \frac{k_1}{k}\cos(kL)}{\cos(kL) + \frac{k_1}{k}\sin(kL)} &= \frac{k_2}{k} \\ \implies \frac{\tan(kL) - \frac{k_1}{k}}{1 + \frac{k_1}{k}\tan(kL)} &= \frac{k_2}{k} \\ \implies \tan(kL) &= \frac{\frac{k_1}{k} + \frac{k_2}{k}}{1 - \frac{k_1}{k}\frac{k_2}{k}} \\ \implies \tan(kL) &= \tan\left(\tan^{-1}\left(\frac{k_1}{k}\right) + \tan^{-1}\left(\frac{k_2}{k}\right)\right) \\ \implies \tan^{-1}\left(\frac{k_1}{k}\right) + \tan^{-1}\left(\frac{k_2}{k}\right) &= kL \pm n\pi \end{aligned}$$

To find the condition for semi-infinite well, we will use $V_1 \to \infty \implies k_1 \to \infty$

$$\begin{aligned} \tan^{-1}\left(\frac{k_2}{k}\right) &= kL \pm (2n' + 1)\frac{\pi}{2} \\ \implies \frac{k_2}{k} &= \cot(kL) \end{aligned}$$

Question 2

Consider a particle of mass m trapped in a finite square box of length a with barrier height equals to V_0 . Find the number of bound states and the corresponding energies for the finite square well potential if $\sqrt{\frac{ma^2V_0}{2\hbar^2}} = 1$

From Quantization equations we have

$$\begin{aligned} \tan\left(\frac{ka}{2}\right) &= \frac{\alpha}{k} \\ -\cot\left(\frac{ka}{2}\right) &= \frac{\alpha}{k} \end{aligned}$$

Where

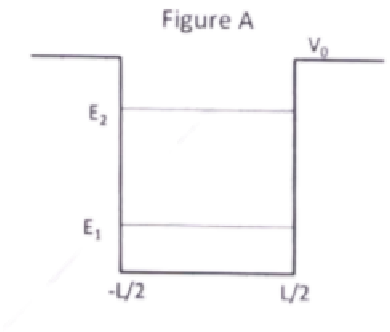
$$\begin{aligned} k^2 &= \frac{2mE}{\hbar^2} \\ \alpha^2 &= \frac{2m}{\hbar^2}(V_0 - E) \end{aligned}$$

From the relation given in question we have $\alpha^2 + k^2 = \frac{4}{a^2} \implies \alpha = \sqrt{\frac{4}{k^2a^2} - 1}$

So we have $\frac{\alpha}{k}$ going to 0 at $ka = 2$ and $\tan\left(\frac{ka}{2}\right)$ has it's first zero at $ka = \pi$. So, we will have only one bound state.

Question 3

An electron is trapped in a 1-dimensional symmetric potential well of height V_0 and width L (Figure A). The energy of electron is E, its wave number inside the well is k, and the magnitude of the wave number outside the well is α.



(a) Derive the energy quantization conditions, in terms of k, α and L, for the symmetric and anti-symmetric bound states.

Symetric Solution:
From TISE:

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} = \begin{cases} \alpha^2 & x < -\frac{L}{2} \\ -k^2 & -\frac{L}{2} \le x \le \frac{L}{2} \\ \alpha^2 & x > L \end{cases}$$

$$\psi(x) = \begin{cases} Ae^{\alpha x} & x < -\frac{L}{2} \\ B\cos(kx) & -\frac{L}{2} \le x \le \frac{L}{2} \\ Ae^{-\alpha x} & x > \frac{L}{2} \end{cases}$$

Continuity and Differentiability at $x = \frac{L}{2}$

$$B\cos\frac{kL}{2} = Ae^{\frac{-\alpha L}{2}}$$
$$-Bk\sin\frac{kL}{2} = -\alpha Ae^{\frac{-\alpha L}{2}}$$

Dividing above two equations $\implies \tan\frac{kL}{2} = \frac{\alpha}{k}$
Anti Symetric Solution:
From TISE:

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} = \begin{cases} \alpha^2 & x < -\frac{L}{2} \\ -k^2 & -\frac{L}{2} \le x \le \frac{L}{2} \\ \alpha^2 & x > L \end{cases}$$

$$\psi(x) = \begin{cases} Ae^{\alpha x} & x < -\frac{L}{2} \\ B\sin(kx) & -\frac{L}{2} \leq x \leq \frac{L}{2} \\ Ae^{-\alpha x} & x > \frac{L}{2} \end{cases}$$

Continuity and Differentiability at $x = \frac{L}{2}$

$$B\sin\frac{kL}{2} = Ae^{\frac{-\alpha L}{2}}$$
$$Bk\cos\frac{kL}{2} = -\alpha Ae^{\frac{-\alpha L}{2}}$$

Dividing above two equations $\Longrightarrow \cot\frac{kL}{2} = -\frac{\alpha}{k}$

(b) When the width of the well is $L = 0.2nm$, it is found that the ground state energy $E_1 = 4.45eV$, and the first excited state energy $E_2 = 15.88eV$. Calculate V_0 .

$$k_1 = \frac{\sqrt{2mE_1}}{\hbar} = 10.64nm^{-1}$$
$$\frac{k_1L}{2} = 1.064\text{radians}$$
$$\tan\frac{k_1L}{2} = 1.8 = \frac{\alpha}{k_1} = \sqrt{\frac{V_0}{E} - 1}$$
$$\Longrightarrow \frac{V_0}{E} = 4.24$$
$$\Longrightarrow V_0 = 18.87eV$$

(c) Calculate the penetration depth for the ground state.

Penetration depth $\delta = \alpha^{-1}$

$$\alpha = 1.8k_1 = 19.152nm^{-1}$$
$$\delta = 0.0522nm$$

(d) If the width of the potential well is doubled to $2L$ keeping V_0 the same, estimate the change in the ground state energy.

Let,

$$L \to L^{'} = 2L$$
$$E_1 \to E_1^{'}$$
$$k_1 \to k_1^{'} = \frac{\sqrt{2mE_1^{'}}}{\hbar}$$

Condition for ground state is $\tan(k_1^{'}L) = \frac{\alpha^{'}}{k_1^{'}}$

$$\begin{aligned}
\tan^2(k_1^{'}L) &= \left(\frac{\alpha^{'}}{k_1^{'}}\right)^2 = \frac{v_0}{E_1^{'}} - 1 \\
\cos(k_1^{'}L) &= \sqrt{\frac{E_1^{'}}{V_0}} \\
&= \frac{\left(\frac{\sqrt{2mE_1^{'}}}{\hbar}\right)L}{\left(\frac{\sqrt{2mV_0}}{\hbar}\right)L} \\
&= \frac{k_1^{'}L}{\text{Constant}} \\
\text{Constant} &= 4.42 = 0.226^{-1}
\end{aligned}$$

Now we have Quantization equation as $\cos(k_1^{'}L) = 0.226(k_1^{'}L)$

$$\begin{aligned}
\cos(k_1^{'}L) &= 0.226(k_1^{'}L) \\
\implies k_1^{'}L &\simeq 0.41\pi \\
\implies (k_1^{'}L)^2 &\simeq (0.41\pi)^2 \\
\implies \frac{2mE_1^{'}}{\hbar^2}L^2 &= (0.41\pi)^2 \\
\implies E_1^{'} &= 1.6eV
\end{aligned}$$

(e) Consider the potential which is generated from Figure A by setting $V = \infty$ at $L = 0$. What is the energy of the ground state in this case?

In this case we need to have $\psi(x) = 0$ at $x = 0$ and they should satisfy the same boundary conditions as before. So we can take bound states of this case are the anti-symmetric states of initial case.
Ground state energy $= 15.88eV$

(f) How many bound states are possible in this case?

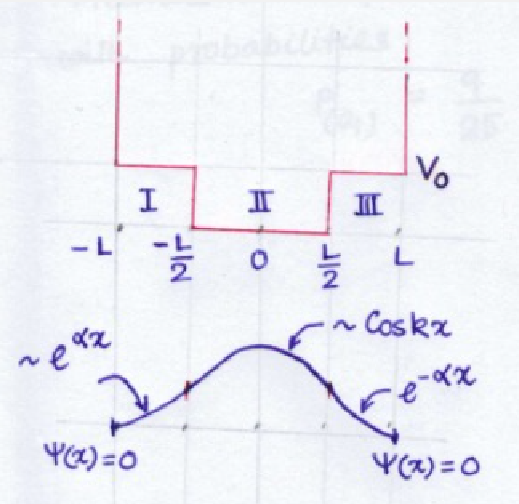
For bound states in this case we need $E < V_0 \implies E < 18.84eV$.
We know that energy of second anti-symmetric state is greater than energy of second symmetric state($\approx 9E_1 = 40eV > V_0(18.84eV)$). So second anti-symmetric can't exist.
Hence, we have only one bound solution.

Question 4

Consider a particle of mass m in a potential given by

$$V(x) = \begin{cases} 0 & |x| < \frac{L}{2} \\ V_0 & \frac{L}{2} < |x| < L \\ \infty & |x| \geq L \end{cases}$$

(a) Sketch the potential and the qualitative nature of the ground-state wave-function (without solving the Schrodinger equation). Mention the functional form of the wave function in each region.



(b) An electron is trapped in a symmetric finite potential of depth $V_0 = 1000eV$ and width $L = 1$. What is approximate energy of the ground state?

$$E \simeq \frac{\pi^2\hbar^2}{2m(L + 2\delta^2)}$$

$$\delta = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

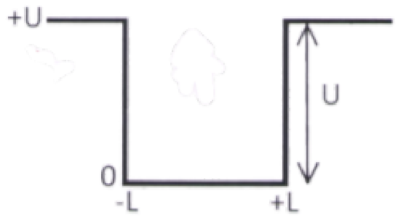
$$\delta \simeq \frac{\hbar}{\sqrt{2mV_0}} = 6.15pm$$

$$\implies E = 29.57eV$$

Here in δ it's ok to drop E term in denominator since $V_0 \gg E$

Question 5

A particle with energy E is bound in a finite square well potential with height U and width $2L$ (as shown in the figure below)



(a) Consider the case $E < U$, obtain the energy quantization condition for the symmetric wave functions in terms of K and α, where $K = \sqrt{\frac{2mE}{\hbar^2}}$ and $\alpha = \frac{2m(U-E)}{\hbar^2}$

From TISE:

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} = \begin{cases} \alpha^2 & x < -L \\ -k^2 & -L \le x \le L \\ \alpha^2 & x > L \end{cases}$$

$$\psi(x) = \begin{cases} Ae^{\alpha x} + Be^{-\alpha x} & x < -L \\ C\cos(kx) + D\sin(kx) & -L \le x \le L \\ Ee^{\alpha x} + Fe^{-\alpha x} & x > L \end{cases}$$

$\psi(x)$ cannot be infinite $\implies B = E = 0$ For symmetric solutions, $\implies A = F, D = 0$
Continuity and Differentiability at $x = L$

$$Ae^{-\alpha L} = C\cos(kL)$$

$$\alpha Ae^{-\alpha L} = kC\sin(kL)$$

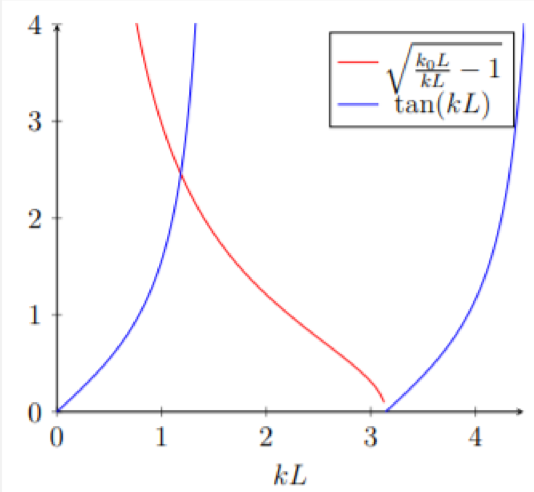
Dividing above equations

$$\tan(kL) = \frac{\alpha}{k}$$

(b) Apply this result to an electron trapped at a defect site in a crystal. Modeling the defect as a finite square well potential with height 5eV and width 200pm, calculate the ground state energy ?

As we know, the ground state is a symmetric one, hence the ground state energy is the lowest k and thus lowest E satisfying $\tan(kL) = \frac{\alpha}{k}$
Writing $k_0 = \frac{\sqrt{2mU}}{\hbar}$, we have $\frac{\alpha}{k} = \sqrt{\frac{k_0^2L^2}{k^2L^2} - 1}$. We also have $k_0L = 2.298$. Thus we can now solve this equation numerically to get $kL = 1.081 \implies E = \frac{\hbar^2(k^2L^2)}{2mL^2} = 1.1eV$

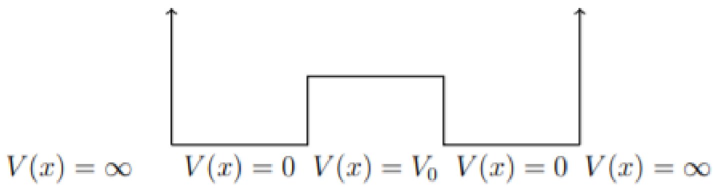
(c) Calculate the total number of bound states with symmetric wavefunction?



As is clear from the picture, as we increase k_0, a new bound state is possible whenever the x intercept of $\sqrt{\frac{k_0L}{kL}-1}$ crosses a multiple of π. Thus the number of bound states is $\lceil \frac{k_0L}{\pi} \rceil = \lceil \frac{\sqrt{2mU}L}{\hbar\pi} \rceil$

Question 6

A particle of mass m is bound in a double well potential shown in the figure. Its energy eigenstate $\psi(x)$ has energy eigenvalue $E = V_0$ (where V_0 is the energy of the plateau in the middle of the potential well). It is known that $\psi(x) = C$ (C is a constant) in the plateau region.



(a) Obtain $\psi(x)$ for the regions $2L < x < L$ and $L < x < 2L$ and the relation between the wavenumber k and L.

From TISE:

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} = \begin{cases} -k^2 & -2L \le x < -L \\ 0 & -L \le x \le L \\ -k^2 & L < x \le 2L \end{cases}$$

$$\psi(x) = \begin{cases} 0 & x < -2L \\ A\cos(kx) + B\sin(kx) & -2L \leq x < -L \\ C & -L \leq x \leq L \\ D\cos(kx) + E\sin(kx) & L \leq x < 2L \\ 0 & x > 2L \end{cases}$$

Where

$$k^2 = \frac{2mE}{\hbar^2}$$

Continuity at $x = -2L$

$$0 = A\cos(2kL) - B\sin(2kL) \tag{3}$$

Continuity and Differentiability at $x = -L$

$$\begin{aligned} A\cos(kL) - B\sin(kL) &= C \\ k(A\sin(kL) + B\cos(kL)) &= 0 \end{aligned} \tag{4}$$

Continuity and Differentiability at $x = L$

$$\begin{aligned} C &= D\cos(kL) + E\sin(kL) \\ 0 &= k(-D\sin(kL) + E\cos(kL)) \end{aligned} \tag{5}$$

Continuity at $x = 2L$

$$D\cos(2kL) + E\sin(2kL) = 0$$

From (3) and (4):

$$\begin{aligned} A\cos(2kL) &= B\sin(2kL) \\ A\sin(kL) &= -B\cos(kL) \\ &\text{Multiplying above equations} \\ \implies AB(\cos(2kL)\cos(kL)) &= -AB(\sin(2kL)\sin(kL)) \\ \implies AB(\cos(kL)) &= 0 \end{aligned} \tag{6}$$

Case(1):

$$\begin{aligned} \cos(kL) &= 0 \\ \implies kL &= (2n+1)\frac{\pi}{2} \\ \text{From 4.2} \implies A &= 0 \end{aligned} \tag{7}$$

Case(2): $AB = 0$ here either A or B can be 0 but not both because $\psi(x)$ cannot be 0 everywhere. $A = 0$ is result of case(1). So we can check only $B = 0$ case here.

$$\begin{aligned} B = \&A! &= 0 \\ \text{From 4 } \implies & A\sin(kL) = 0 \\ \implies \sin(kL) &= 0 \\ \text{From 3} \implies & A = 0 \\ \implies & A = B = 0 \end{aligned} \tag{8}$$

Contradiction, not a valid solution.

$$\psi(x) = \begin{cases} 0 & x < -2L \\ -C(-1)^n \sin(kx) & -2L \leq x < -L \\ C & -L \leq x \leq L \\ C(-1)^n \sin(kx) & L \leq x < 2L \\ 0 & x > 2L \end{cases}$$

$$kL = (2n+1)\frac{\pi}{2}$$

(b) Determine C in terms of L

$$\int |\psi(x)|^2 = 1$$
$$\implies C = \frac{1}{\sqrt{3L}}$$

(c) Assume that the bound particle is an electron and $L = 1A$. Calculate the 2 lowest values of V_0 (in eV) for which such a solution exists.

As solved above, the necessary and sufficient condition for such a solution to exist is $\frac{\sqrt{2mV_0}}{\hbar}L = \frac{(2n+1)\pi}{2}$

$$\implies V_0 = \frac{(2n+1)^2\pi^2\hbar^2}{8mL^2}$$

Thus the two lowest values of V_0 are obtained by putting $n = 0$ and $n = 1$, giving us $V_0 = 9.34eV, V_0 = 84eV$

(d) For the smallest allowed k, calculate the expectation values for x, x^2, p and p^2 and show that Heisenberg's Uncertainty Relation is obeyed.

The smallest allowed value of k is for $n = 0$

$$\psi(x) = \begin{cases} 0 & x < -2L \\ -\sqrt{\frac{1}{3L}} \sin(kx) & -2L \leq x < -L \\ \sqrt{\frac{1}{3L}} & -L \leq x \leq L \\ \sqrt{\frac{1}{3L}} \sin(kx) & L \leq x < 2L \\ 0 & x > 2L \end{cases}$$

$$\begin{aligned}\langle x\rangle &= \int_{-2L}^{-L}\frac{1}{3L}x\sin^2\left(\frac{\pi x}{2L}\right)dx + \int_{-L}^{L}\frac{1}{3L}xdx + \int_{L}^{2L}\frac{1}{3L}x\sin^2\left(\frac{\pi x}{2L}\right)dx \\ &= 0 \\ \langle x^2\rangle &= \int_{-2L}^{-L}\frac{1}{3L}x^2\sin^2\left(\frac{\pi x}{2L}\right)dx + \int_{-L}^{L}\frac{1}{3L}x^2dx + \int_{L}^{2L}\frac{1}{3L}x^2\sin^2\left(\frac{\pi x}{2L}\right)dx\end{aligned}$$

$$2L^2\left(\frac{1}{2}-\frac{1}{\pi^2}\right)$$

$$\begin{aligned}\langle p\rangle &= \int -i\hbar\frac{d\psi}{dx} \\ &= 0 \\ \langle p^2\rangle &= \int \hbar^2\frac{d^2\psi(x)}{dx^2} \\ &= \frac{\pi^2\hbar^2}{12L^2}\end{aligned}$$

$$\begin{aligned}\Delta x &= \sqrt{\langle x^2\rangle - \langle x\rangle^2} \\ \Delta p &= \sqrt{\langle p^2\rangle - \langle p\rangle^2} \\ \Delta x\Delta p &= \sqrt{\frac{\pi^2}{12}-\frac{\hbar}{6}} = 0.81\hbar > 0.5\hbar\end{aligned}$$