

Assignment 1: Blackbody Radiation

1. If the absolute temperature of a black body is increased from T to $1.414T$, by what factor is the total emitted power per unit area (R_T) increased? (Use Stefan's law.)
2. Derive the value of the constant A in the Wien's displacement law,

$$\lambda_{\max}T = A, \quad (1)$$

where λ_{\max} as the wavelength at which the spectral radiance is maximum.

3. A particular radiating cavity has the maximum of its spectral distribution of radiated power at a wavelength of $27 \mu\text{m}$ (Infrared Region). The temperature is then changed so that the total power radiated by the cavity is 16 times higher. At what wavelength does the new spectral distribution have its maximum value? (Use Stefan's and Wien's displacement laws.)
4. Find the energy density of black body radiation at $T = 6000 \text{ K}$ in the range from 450 to 460 nm, assuming that this range is so narrow that the energy density function $\rho_T(f)$ does not vary much over it. (Use Planck's radiation law.)
5. (a) Show that the expression for the number of standing waves can also be expressed in terms of wavelength and written as,

$$N(\lambda) d\lambda = \frac{8\pi V d\lambda}{\lambda^4}, \quad (2)$$

where $V = L^3$ is the volume of the cubic cavity.

- (b) How many independent standing waves with wavelengths between 9.5 and 10.5 mm are present in a cubical cavity 1 m on a side?
6. Assuming that the energies of the radiation modes inside a cavity are discrete and equal to $E_n = nhf$, prove the relationship,

$$\frac{\sum_{n=0}^{\infty} E_n p(E_n)}{\sum_{n=0}^{\infty} p(E_n)} = \frac{hf}{\exp(hf/kT) - 1}, \quad (3)$$

where $p(E)$ is the Boltzmann distribution function.

7. Show that for very large wavelengths λ , Planck's formula for spectral radiance,

$$\rho(\lambda) = \frac{8\pi hc}{\lambda^5} \frac{1}{\exp(hc/\lambda kT) - 1}, \quad (4)$$

reduces to the Rayleigh-Jeans formula,

$$\rho(\lambda) = \frac{8\pi}{\lambda^4} kT. \quad (5)$$

(Note that Rayleigh-Jeans or Planck's formulas can express the spectral densities either in terms of frequency or wavelength. Refer to the approach followed in Question 5.)

8. A tuning fork has a natural frequency of 500 Hz and its total vibrational energy is 0.04 J. An atom emits orange light at a frequency of 5.00×10^{14} Hz and has an energy of 2.0 eV. Which of these systems is more likely to exhibit quantum graininess? Support your answer quantitatively.

Blackbody Radiation:**Answer 1.**

Using Stefan's law,

$$R_T = \sigma T^4$$

For the first body,

$$R_1 = \sigma T_1^4$$

For the second body,

$$R_2 = \sigma T_2^4$$

$$\frac{R_2}{R_1} = \frac{\sigma T_2^4}{\sigma T_1^4}$$

$$\frac{R_2}{R_1} = \left(\frac{T_2}{T_1}\right)^4$$

but it is given that,

$$T_2 = 1.414 T_1$$

So,

$$\frac{R_2}{R_1} = \left(\frac{1.414 T_1}{T_1}\right)^4$$

$$\frac{R_2}{R_1} = (1.414)^4$$

This implies,

$$R_2 = 4 R_1.$$

i.e. the total emitted power R_T increases by a factor of 4.

Answer 2.

In Wien's displacement law, $\lambda_{\max} \times T = A$, we have to find the value of A.

Solution set 1: Blackbody radiation

Since $f = c/\lambda$, we have $|df| = |df/d\lambda|d\lambda = (c/\lambda^2)d\lambda$; we can thus write Plank's energy density in terms of wavelength as follows,

$$\rho(\lambda) = \rho(f) \left| \frac{df}{d\lambda} \right| = \frac{8\pi hc}{\lambda^5} \frac{1}{\exp\left(\frac{hc}{\lambda k T}\right) - 1}.$$

The maximum of $\rho(\lambda)$ corresponds to $\partial\rho(\lambda)/\partial\lambda = 0$.

$$\begin{aligned} \frac{d\rho}{d\lambda} &= 8\pi hc \frac{d}{d\lambda} \left[\lambda^{-5} \cdot \left(\exp\left(\frac{hc}{\lambda k T}\right) - 1 \right)^{-1} \right] \\ &= 8\pi hc (-5) \lambda^{-6} \left(\exp\left(\frac{hc}{\lambda k T}\right) - 1 \right)^{-1} + \frac{8\pi hc}{\lambda^5} (-1) \left(\exp\left(\frac{hc}{\lambda k T}\right) - 1 \right)^{-2} \exp\left(\frac{hc}{\lambda k T}\right) \left(\frac{hc}{k T} \right) \frac{-1}{\lambda^2} \\ &= \frac{8\pi hc}{\lambda^6} \left[\frac{-5}{\exp\left(\frac{hc}{\lambda k T}\right) - 1} + \left(\frac{hc}{\lambda k T} \right) \frac{\exp\left(\frac{hc}{\lambda k T}\right)}{\left(\exp\left(\frac{hc}{\lambda k T}\right) - 1 \right)^2} \right] \\ &= \frac{8\pi hc}{\lambda^6} \left[\frac{-5 \left(1 - \exp\left(\frac{-hc}{\lambda k T}\right) \right) \exp\left(\frac{hc}{\lambda k T}\right)}{\left(\exp\left(\frac{hc}{\lambda k T}\right) - 1 \right)^2} + \left(\frac{hc}{\lambda k T} \right) \frac{\exp\left(\frac{hc}{\lambda k T}\right)}{\left(\exp\left(\frac{hc}{\lambda k T}\right) - 1 \right)^2} \right] \end{aligned}$$

Taking the terms common,

$$= \frac{8\pi hc}{\lambda^6} \left[-5 \left(1 - \exp\left(\frac{-hc}{\lambda k T}\right) \right) + \frac{hc}{\lambda k T} \right] \frac{\exp\left(\frac{hc}{\lambda k T}\right)}{\left(\exp\left(\frac{hc}{\lambda k T}\right) - 1 \right)^2}.$$

Since $\frac{d\rho}{d\lambda}|_{\lambda=\lambda_{max}} = 0$, So,

$$\frac{8\pi hc}{\lambda^6} \left[-5 \left(1 - \exp\left(\frac{-hc}{\lambda k T}\right) \right) + \frac{hc}{\lambda k T} \right] \frac{\exp\left(\frac{hc}{\lambda k T}\right)}{\left(\exp\left(\frac{hc}{\lambda k T}\right) - 1 \right)^2} = 0.$$

Equating the coefficients with zero, only the term inside square bracket can be made zero,

$$-5 \left(1 - \exp\left(\frac{-hc}{\lambda k T}\right) \right) + \frac{hc}{\lambda k T} = 0$$

Let $a = \frac{hc}{\lambda k T}$,

$$-5 \left(1 - \exp\left(\frac{-a}{\lambda}\right) \right) + \frac{a}{\lambda} = 0$$

$$\frac{a}{\lambda} = 5 \left(1 - \exp\left(\frac{-a}{\lambda}\right) \right)$$

We can solve this transcendental equation either graphically or numerically.

Let's write $\frac{a}{\lambda} = 5 - \epsilon$

$$5 - \epsilon = 5 - 5 \exp(-5 + \epsilon)$$

$$\epsilon \approx 5 \exp(-5) \approx 0.0337 .$$

Therefore,

$$\frac{a}{\lambda} = 5 - 0.0337 = 4.9663$$

Since $a = \frac{hc}{kT}$, it becomes,

$$\frac{hc}{\lambda kT} = 4.9663$$

$$\lambda_{max} \times T = \frac{1}{4.9663} \frac{hc}{k}$$

$$\lambda_{max} \times T = 2.89 \times 10^{-3} mK .$$

This is the Required Result.

Answer 3.

Given is $\lambda_{max} = 27\mu m$.

For the first body,

$$R_1 = \sigma T_1^4 . \tag{1}$$

For the second body,

$$R_2 = \sigma T_2^4 .$$

But it is given that,

$$R_2 = 16 R_1 .$$

This implies that,

$$16R_1 = \sigma T_2^4 .$$

Substituting R_1 from Eq.(1),

$$16 \sigma T_1^4 = \sigma T_2^4$$

$$T_2^4 = 16 T_1^4.$$

We get,

$$T_2 = 2 T_1. \tag{2}$$

Now, using the Wien's displacement law,

$$\begin{aligned} \lambda_{1max} &= \frac{A}{T_1} & \lambda_{2max} &= \frac{A}{T_2} \\ T_1 &= \frac{A}{\lambda_{1max}} & T_2 &= \frac{A}{\lambda_{2max}} \end{aligned}$$

Putting it in the above expression (2),

$$\frac{A}{\lambda_{2max}} = 2 \frac{A}{\lambda_{1max}}$$

$$\lambda_{2max} = \frac{1}{2} \lambda_{1max}$$

$$\lambda_{2max} = 13.5 \mu\text{m}.$$

This is the required result.

Answer 4.

Given is $T = 6000 \text{ K}$, $\lambda_{min} = 450 \text{ nm}$, $\lambda_{max} = 460 \text{ nm}$, $\rho_T(f) = ?$

$$f_{min} = \frac{c}{\lambda_{max}} = \frac{3 \times 10^8}{460 \times 10^{-9}} = 6.52 \times 10^{14} \text{ Hz}$$

$$f_{max} = \frac{c}{\lambda_{min}} = \frac{3 \times 10^8}{450 \times 10^{-9}} = 6.66 \times 10^{14} \text{ Hz}$$

$$\Delta f = f_{max} - f_{min} = 1.45 \times 10^{13} \text{ Hz}$$

$$f_{avg} = \frac{f_{min} + f_{max}}{2} = 6.60 \times 10^{14} \text{ Hz}.$$

Solution set 1: Blackbody radiation

To use Plank's formula, we first evaluate $\frac{hf_{avg}}{kT}$, assuming the frequency in the interval is the average value,

$$\frac{hf_{avg}}{kT} = \frac{(6.63 \times 10^{-34} \text{ J}\cdot\text{sec})(6.60 \times 10^{14} \text{ Hz})}{(1.38 \times 10^{-23} \text{ J/K}) 6000 \text{ K}} = 5.28$$

$$\exp(5.28) \approx 197.$$

Plank's radiation formula is

$$\rho_T(f) df = \frac{8 \pi h f}{c^3} \frac{f^2 \Delta f}{\exp(\frac{hf_{avg}}{kT} - 1)}$$

Substituting values,

$$= \frac{(8\pi) (6.63 \times 10^{-34} \text{ J}\cdot\text{sec}) (6.60 \times 10^{14} \text{ Hz})^3 (1.45 \times 10^{13} \text{ Hz})}{(3 \times 10^8)^2 (197 - 1)}$$

$$\rho_T(f) df = 8.2 \times 10^{-7} \text{ J/m}^3.$$

This is the Required result.

Answer 5. Part(a)

The number of standing waves in the cavity (in terms of frequency) is given by,

$$N(f) df = \frac{8 \pi V}{c^3} f^3 df$$

Where $V = a^3$. , Since,

$$f = \frac{c}{\lambda} = c \lambda^{-1}$$
$$df = \frac{-c}{\lambda^2} d\lambda.$$

The negative sign shows that λ decreases when f increases. Since we are concerned with just the scalars, we consider only the magnitude,

$$N(\lambda) d\lambda = \frac{8 \pi V}{c^3} \left(\frac{c^2}{\lambda^2}\right) \left(\frac{c}{\lambda^2}\right) d\lambda$$

$$N(\lambda) d\lambda = \frac{8 \pi V}{\lambda^4} d\lambda \quad (3)$$

This is the required expression for the number of standing waves in terms of wavelength.

Part(b).

Given is $\lambda_{min} = 9.5 \text{ mm}$ $\lambda_{max} = 10.5 \text{ mm}$.

So, $\lambda = \frac{(\lambda_{min} + \lambda_{max})}{2} = 10 \text{ mm}$

and similarly $\Delta\lambda = 1 \text{ mm}$

Substituting values in expression 3,

$$\begin{aligned} N(\lambda) \Delta\lambda &= \frac{8 \pi (1 \text{ m})^3 (10^{-3} \text{ m})}{(10 \times 10^{-3} \text{ m})^4} \\ &= \frac{8 \pi 10^{-3} \text{ m}^4}{10^{-8} \text{ m}^4} \\ &= 8 \pi 10^{8-3} = 8 \pi 10^5 = 2.5 \times 10^6. \end{aligned}$$

Answer 6.

The energy inside the cavity is given by $E_n = nhf$ and the expression for Boltzmann distribution is $P(E) = (\exp(\frac{-E}{kT}))/kT$. Substituting values in the given expression, we get,

$$\frac{\sum_{n=0}^{\infty} E_n P(E_n)}{\sum_{n=0}^{\infty} P(E_n)} = \frac{\sum_{n=0}^{\infty} \frac{nhf}{kT} \exp\left(\frac{-nhf}{kT}\right)}{\sum_{n=0}^{\infty} \frac{1}{kT} \exp\left(\frac{-nhf}{kT}\right)} = kT \frac{\sum_{n=0}^{\infty} na \exp(-na)}{\sum_{n=0}^{\infty} \exp(-na)} \quad (4)$$

Where $a = \frac{hf}{kT}$.

By using the following results, we can simplify it further,

$$\frac{d}{da} \sum_{n=0}^{\infty} \exp(-na) = \sum_{n=0}^{\infty} \frac{d}{da} \exp(-na) = \sum_{n=0}^{\infty} (-n) \exp(-na)$$

Therefore, Numerator of equation (4) becomes,

$$\begin{aligned} \sum_{n=0}^{\infty} na \exp(-na) &= a \sum_{n=0}^{\infty} n \exp(-na) = (-a) \sum_{n=0}^{\infty} (-n) \exp(-na) \\ &= (-a) \frac{d}{da} \sum_{n=0}^{\infty} \exp(-na) \end{aligned} \quad (5)$$

Now,

$$\sum_{n=0}^{\infty} \exp(-na) = 1 + \exp(-a) + \exp(-2a) + \exp(-3a) + \dots$$

$$= 1 + X + X^2 + X^3 + \dots$$

Where $X = \exp(-a)$, But,

$$(1 - X)^{-1} = 1 + X + X^2 + X^3 + \dots$$

So, (5) will become,

$$\begin{aligned} (-a) \frac{d}{da} \sum_{n=0}^{\infty} \exp(-na) &= (-a) \frac{d}{da} \frac{1}{(1 - \exp(-a))} \\ &= (-a) \frac{(-1)(-1)(-1) \exp(-a)}{(1 - \exp(-a))^2} \\ &= a \frac{\exp(-a)}{(1 - \exp(-a))^2} \end{aligned}$$

Similarly, denominator term of equation (4) will be,

$$\sum_{n=0}^{\infty} \exp(-na) = \frac{1}{(1 - \exp(-a))}$$

Using these results, equation (4) will become,

$$\begin{aligned} kT \frac{\sum_{n=0}^{\infty} na \exp(-na)}{\sum_{n=0}^{\infty} \exp(-na)} &= kT \cdot a \cdot \exp(-a) \frac{(1 - \exp(-a))}{(1 - \exp(-a))^2} \\ &= kT \cdot a \cdot \frac{\exp(-a)}{(1 - \exp(-a))} = \frac{kT \cdot a}{\exp(a) - 1} = \frac{hf}{\exp\left(\frac{hf}{kT}\right) - 1} \end{aligned}$$

This is the required proof.

Answer 7.

Plank's radiation formula is given by,

$$\rho_T(\lambda) = \frac{8 \pi hc}{\lambda^5} \frac{1}{\exp\left(\frac{hc}{\lambda kT}\right) - 1} \quad (6)$$

Let $x = \frac{hc}{\lambda kT}$. For very large value of λ , $x \ll 1$.

So we can write it as,

$$\exp(x) \approx 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} \dots$$

$$\exp\left(\frac{hc}{\lambda kT}\right) - 1 = \left(1 + \frac{hc}{\lambda kT} + \dots\right) - 1 \approx \frac{hc}{\lambda kT}.$$

Hence the expression (4) becomes,

$$\rho_T(\lambda) = \frac{8 \pi hc}{\lambda^5} \frac{\lambda kT}{hc}$$

$$\rho_T(\lambda) = \frac{8 \pi kT}{\lambda^4}.$$

This is the required result.

Answer 8

For the tuning fork,

$$h f_1 = (6.63 \times 10^{-34} \text{ J}\cdot\text{sec}) (500 \text{ sec}^{-1}) = 2.315 \times 10^{-31} \text{ J}$$

The total energy of the vibrating tuning fork is therefore about 10^{29} times the quantum energy hf . The quantization of energy is obviously too small to be observed. That's why, we say that tuning fork is appearing to obey classical physics.

For the atomic oscillator,

$$h f_2 = (6.63 \times 10^{-34} \text{ J}\cdot\text{sec}) (5 \times 10^{14} \text{ sec}^{-1}) = 3.32 \times 10^{-19} \text{ J}$$

In electronvolts (eV),

$$h f_2 = \frac{3.32 \times 10^{-19} \text{ J}}{1.60 \times 10^{-19} \text{ J/eV}} = 2.8 \text{ eV}$$

This is a significant amount of energy on an atomic scale and it is not surprising that classical physics fails to explain it. Quantum behavior will be dominant here.

Assignment 2: Photoelectric effect, Compton effect, X-rays

1. A hydrogen atom is excited from a state with $n = 1$ to one with $n = 4$. Calculate the energy that must be absorbed by the atom? Calculate and display on an energy-level diagram the different photon energies that may be emitted if the atom returns to $n = 1$ state?
2. Light of wavelength 200 nm falls on an aluminium surface, having work function 4.2 eV. What is the K.E. of the fastest emitted photoelectron? Also find the stopping potential and cutoff wavelength for Al.
3. When a photon energy is increased from hf to $2hf + w_0$, what is the increase in the saturation photoelectric current?
4. Why does the photoelectric current not rise vertically to its maximum value when the applied potential difference is slightly more positive than $-V_0$?
5. Do you observe Compton effect with visible light? Why or why not?
6. How many collisions does a photon require to lose its energy completely (that is, to disappear), in Compton scattering and in photoelectric effect?
7. Find the shortest wavelength present in the radiation from an X-ray machine whose accelerating potential is 50,000 V.
8. X-rays of wavelength 10 pm are scattered from a target. Find (a) the wavelength of the X-rays scattered through an angle of 45° , (b) the maximum wavelength present in the scattered X-rays, (c) the maximum K.E. of the recoil electrons.
9. The relativistic expression for kinetic energy should be used for the electron in the photoelectric effect when $v/c > 0.1$, if errors greater than about 1 percent are to be avoided. For photoelectrons ejected from an aluminum surface ($w_0 = 4.2$ eV), what is the smallest wavelength of an incident photon for which the non-relativistic expression may be used?
10. Derive a relation between the kinetic energy K of the recoil electron and the energy E of the incident photon in the Compton effect. One form of the relation is

$$\frac{K}{E} = \frac{\left(\frac{2hf}{m_0c^2}\right) \sin^2 \frac{\theta}{2}}{1 + \left(\frac{2hf}{m_0c^2}\right) \sin^2 \frac{\theta}{2}}$$

11. Photons passing through the pupil are focused by the lens onto the retina and are detected by two types of photosensitive cells, called rods and cones. Rods are highly sensitive photoreceptors with a peak response at the wavelength 510 nm. They do not register colour, but they are responsible for our vision under dimmed light conditions, which is termed scotopic vision. Cones are color sensitive and are responsible for our day time vision, called photopic vision. There are three types of cone photoreceptors, which are sensitive to the blue, green, and red wavelengths: 430 nm, 535 nm, and 575 nm, respectively. All three cones have an overall peak response of 555 nm.
- (a) Calculate the photon energy (in eV) for the peak responsivity of each photoreceptor in the eye.
- (b) The fovea is a region in the retina lying on the visual axis; images are focused onto this region. The density of the cones in the fovea is on the order of 150,000/m². Below a light intensity of about 100 uW m², cones are not functional and rods take over the vision.
- (c) What is the minimum photon flux for color vision?
- (d) If a visual sensation persists for a time (1/5)th of a second, how many photons does the eye need per cone for a visual color sensation?
- (e) If the eye is 10 percent efficient overall, due to photon reflections, etc., how many photons are actually absorbed per cone to generate a colored visual sensation?

Photoelectric effect, Compton effect, X-raysAnswer 1.

The maximum K.E. of photoelectrons is equal to the energy of photons minus the work function of metal. So, for red light ($\lambda = 650$) nm,

$$(K.E)_{max} = E - w_o \quad (1)$$

$$\begin{aligned} E &= hf = \frac{hc}{\lambda} \\ hc &= (6.63 \times 10^{-34} \text{ J sec}) (3 \times 10^8 \text{ m sec}) \\ &= 1.989 \times 10^{-25} \text{ J m} \end{aligned} \quad (2)$$

In terms of electron volts,

$$\begin{aligned} hc &= 1.989 \times 10^{-25} \text{ J.m} \times \frac{1\text{eV}}{1.6 \times 10^{-19} \text{ J}} \\ &= 1243 \text{ eV nm} \end{aligned}$$

Substituting values in Eq.(2), we get

$$\begin{aligned} E &= hf = \frac{hc}{\lambda} = \frac{1243 \text{ eV nm}}{650 \text{ nm}} \\ &= 1.91 \text{ eV} \end{aligned}$$

If the difference between energy (E) and the workfunction (w_o) is equal to zero or positive (from equation (1)), only then will the photoelectric effect will take place. The only metal that satisfies this requirement is cesium having a workfunction $w_o = 1.9$ eV.

Similarly, for green light,

$$\begin{aligned} E &= \frac{hc}{\lambda} = \frac{1240 \text{ eV nm}}{450 \text{ nm}} \\ &= 2.75 \text{ eV} \end{aligned}$$

In this case, the metals we can use are, lithum (2.3 eV), barium (2.5 eV) and cesium (1.9 eV).

Answer 2.

Given is $\lambda = 200 \text{ nm}$, $(K.E)_{max} = ?$

Using the equation,

$$\begin{aligned}(K.E)_{max} &= hf - w_o \\ &= \frac{hc}{\lambda} - w_o \\ &= \frac{1240 \text{ eV nm}}{200 \text{ nm}} - 4.2 \text{ eV} \\ &= 6.2 \text{ eV} - 4.2 \text{ eV}\end{aligned}$$

$$(K.E)_{max} = 2 \text{ eV}$$

(b)

$$\begin{aligned}(K.E)_{max} &= e V_s \\ V_s &= \frac{(K.E)_{max}}{e} = 2 \text{ V}\end{aligned}$$

(c) Cutoff wavelength is the longest possible wavelength of a photon that will still result in the photoelectric effect occurring. The wavelength is

$$\begin{aligned}E_{min} &= hf_{min} = \frac{hc}{\lambda_{max}} = w_o \\ \lambda_{max} &= \frac{hc}{w_o} \\ &= \frac{1240 \text{ eV nm}}{4.2 \text{ eV}} \\ \lambda_{max} &= 295 \text{ nm}\end{aligned}$$

Answer 3.

$$\begin{aligned}(K.E)_{max} &= \text{Energy of incident photon} - w_o \\ &= (2hf + w_o) - w_o \\ (K.E)_{max} &= 2hf\end{aligned}$$

Since the photoelectric current is proportional to light intensity rather than its frequency, the saturation photocurrent will remain the same.

Answer 4.

The electric field is not strong enough to ensure that all the ejected electrons reach the anode, therefore the current does not immediately rise to its saturation value. Second, there is

a cloud of freshly ejected electrons surrounding the cathode, called the space charge, which prevents the transport of electrons due to repulsive forces. As the voltage is increased, the space charge density decreases allowing more and more electrons to reach the cathode.

Answer 5.

Yes, the Compton effect can occur with visible light. However, the effect may be too small to be observable. The photons for visible light have small energies compared to X-rays. For example, a 500 nm photon will have an energy of 2 eV, five orders of magnitude smaller than the electron rest mass energy of 500 KeV. By energy conservation, the photon energy goes into the kinetic energy of the scattered photon and its own energy after scattering. These energies are, consequently, very small and difficult to measure beyond the experimental uncertainties. In other words, the change in wavelength of the photon and the kinetic energy gained by the electron will be too small to be noticeable.

Answer 6.

In the photoelectric effect, a photon requires just a single collision to completely disappear while in Compton scattering, it requires an infinite number of collisions to lose all of its energy.

Answer 7.

The incident K.E. of the electrons is eV_o . As the electrons are suddenly brought to a halt, all of this energy is radiated as photons. These photons have the minimum wavelength (maximum energy) possible. Therefore,

$$\begin{aligned}\frac{hc}{\lambda_{min}} &= eV_o \\ \lambda_{min} &= \frac{hc}{eV_o} \\ &= \frac{1240 \text{ V nm}}{V_o} \\ &= \frac{1.240 \times 10^{-6} \text{ V m}}{5.0 \times 10^4 \text{ V}} \\ \lambda_{min} &= 2.48 \times 10^{-11} \text{ m} \\ &= 0.02 \text{ nm}\end{aligned}$$

The frequency corresponding to this wavelength will be,

$$\begin{aligned}f_{max} &= \frac{c}{\lambda_{min}} = \frac{3 \times 10^8 \text{ m/sec}}{2.48 \times 10^{-11} \text{ m}} \\ &= 1.2 \times 10^{19} \text{ Hz}\end{aligned}$$

Answer 8.

Given is $\lambda = 10 \text{ pm}$, $\theta = 45^\circ$, $\lambda' = ?$

Using the Compton's scattering formula,

$$\begin{aligned}\lambda' - \lambda &= \lambda_c(1 - \cos \theta) \\ \lambda' &= \lambda + \frac{h}{mc}(1 - \cos \theta) \\ \lambda' &= 10 \text{ pm} + \frac{6.63 \times 10^{-34} \text{ J sec}}{(9.11 \times 10^{-31} \text{ Kg}) (3 \times 10^8 \text{ m/sec})}(1 - \cos 45^\circ) \\ \lambda' &= 10 \text{ pm} + (2.426 \text{ pm}) (0.293) \\ \lambda' &= 10.7 \text{ pm}\end{aligned}$$

(b) $\lambda' - \lambda$ will be maximum when $(1 - \cos \theta)$ is maximum.

When $\theta = \pi$, $(1 - \cos \theta) = 2$, therefore

$$\begin{aligned}\lambda' &= \lambda + \lambda_c(2) \\ &= 10 \text{ pm} + (2.426 \text{ pm})(2) \\ \lambda' &= 14.9 \text{ pm}\end{aligned}$$

$$\begin{aligned}(c) (K.E)_{max, recoil} &= hf - hf' \\ &= hc \left(\frac{1}{\lambda} - \frac{1}{\lambda'} \right) \\ &= (6.63 \times 10^{-34} \text{ J sec}) (3 \times 10^8 \text{ m/sec}) \left(\frac{1}{10 \times 10^{-12} \text{ m}} - \frac{1}{14.9 \times 10^{-12} \text{ m}} \right) \\ &= 6.54 \times 10^{-15} \text{ J} \\ &= 40.8 \text{ KeV}\end{aligned}$$

Answer 9.

Given is $v = 0.1 c$, first we will find out the kinetic energy using the classical result,

$$\begin{aligned}K_{classical} &= \frac{1}{2} m_o v^2 \\ &= \frac{1}{2} m_o (0.1)^2 c^2 \\ &= \frac{1}{2} m_o c^2 \times 0.01 \\ &= 4.1 \times 10^{-16} \text{ J}\end{aligned}$$

If $K < K_{classical}$, the errors are less than 1 percent. For such a case, the wavelength can be calculated as,

$$\begin{aligned}
 hf &= K_{classical} + w_o \\
 \frac{hc}{\lambda} &= K_{classical} + w_o \\
 \lambda &= \frac{hc}{K_{classical} + w_o} \\
 &= \frac{(6.63 \times 10^{-34} \text{ J}\cdot\text{sec}) (3 \times 10^8 \text{ m/sec})}{(4.1 \times 10^{-16} \text{ J}) + (4.2 \times 1.6 \times 10^{-19} \text{ J})} \\
 \lambda &= 4.84 \text{ \AA}
 \end{aligned}$$

Answer 10.

Kinetic energy of recoil electron = K

Energy of incident photon = E

Energy of final photon = E'

Using the law of conservation of energy,

$$\begin{aligned}
 E &= E' + K \\
 K &= E - E'
 \end{aligned} \tag{3}$$

To find $E' = hf'$, we use the equation,

$$\begin{aligned}
 \lambda' - \lambda_o &= \frac{c}{f'} - \frac{c}{f_o} = \frac{h}{m_o c} (1 - \cos \theta) \\
 \frac{c}{f'} &= \frac{h}{m_o c} (1 - \cos \theta) + \frac{c}{f_o} \\
 &= \frac{hf_o (1 - \cos \theta) + m_o c^2}{m_o c v_o} \\
 \frac{f'}{c} &= \frac{m_o c f_o}{hf_o (1 - \cos \theta) + m_o c^2} \\
 f' &= \frac{m_o c^2 f_o}{hf_o (1 - \cos \theta) + m_o c^2} \\
 hf' &= \frac{m_o c^2 (hf_o)}{hf_o (1 - \cos \theta) + m_o c^2} \\
 &= \frac{m_o c^2}{(1 - \cos \theta) + \frac{m_o c^2}{hf_o}}
 \end{aligned}$$

$$\text{Let } x = \frac{hf_o}{m_o c^2}$$

$$\text{Energy of final photon} = hf' = \frac{m_0c^2}{(1 - \cos \theta) + \frac{1}{x}}$$

using equation (4),

$$\begin{aligned} K &= hf_o - hf' \\ &= hf_o - \frac{m_0c^2}{(1 - \cos \theta) + \frac{1}{x}} \\ &= \left(\frac{hf_o}{m_0c^2} \right) m_0c^2 - \frac{m_0c^2}{(1 - \cos \theta) + \frac{1}{x}} \\ &= x m_0c^2 - \frac{m_0c^2}{(1 - \cos \theta) + \frac{1}{x}} \\ &= m_0c^2 \left(x - \frac{1}{(1 - \cos \theta) + \frac{1}{x}} \right) \\ &= m_0c^2 \left(x - \frac{x}{1 + x(1 - \cos \theta)} \right) \\ &= m_0c^2 \left(\frac{x^2 (1 - \cos \theta)}{1 + x(1 - \cos \theta)} \right) \\ &= m_0c^2 \left(\frac{x x (1 - \cos \theta)}{1 + x(1 - \cos \theta)} \right) \\ &= m_0c^2 \left(\frac{\frac{hf_o}{m_0c^2} x (1 - \cos \theta)}{1 + x(1 - \cos \theta)} \right) \\ &= hf_o \left(\frac{x (1 - \cos \theta)}{1 + x(1 - \cos \theta)} \right). \end{aligned}$$

Since $E = hf_o$,

$$\begin{aligned} \frac{K}{E} &= \left(\frac{x (1 - \cos \theta)}{x(1 - \cos \theta) + 1} \right) \\ \frac{K}{E} &= \left(\frac{x (2 \sin^2(\frac{\theta}{2}))}{1 + x(2 \sin^2(\frac{\theta}{2}))} \right) \\ \frac{K}{E} &= \frac{\left(\frac{2hf_o}{m_0c^2} \right) \sin^2(\frac{\theta}{2})}{1 + \left(\frac{2hf_o}{m_0c^2} \right) \sin^2(\frac{\theta}{2})}. \end{aligned}$$

This is the required proof .

Problem # 11. (There were some typing mistakes in the posted questions; following is the correct wording).

Photons passing through the pupil are focused by the lens onto the retina and are detected by two types of photosensitive cells, called rods and cones. Rods are highly sensitive photoreceptors with a peak response at the wavelength 510 nm. They do not register colour, but they are responsible for our vision under dimmed light conditions, which is termed sco-

topic vision. Cones are color sensitive and are responsible for our day time vision, called photopic vision. There are three types of cone photoreceptors, which are sensitive to the blue, green, and red wavelengths: 430 nm, 535 nm, and 575 nm, respectively. All three cones have an overall peak response of 555 nm.

(a) Calculate the photon energy (in eV) for the peak responsivity of each photoreceptor in the eye. The fovea is a region in the retina lying on the visual axis; images are focused onto this region. The density of the cones in the fovea is on the order of $150,000/\text{mm}^2$. Below a light intensity of about $100 \mu\text{W}/\text{m}^2$, cones are not functional and rods take over the vision.

(b) What is the minimum photon flux for color vision?

(c) If a visual sensation persists for a time $(1/5)$ th of a second, how many photons does the eye need per cone for a visual color sensation?

(d) If the eye is 10 percent efficient overall, due to photon reflections, etc., how many photons are actually absorbed per cone to generate a colored visual sensation?

Answer 11.

Photon energies for cone photoreceptors can be calculated as follows,

For blue light,

$$\begin{aligned} E &= hf = \frac{hc}{\lambda} = \frac{1243 \text{ eV nm}}{430 \text{ nm}} \\ &= 2.89 \text{ eV} \end{aligned}$$

For green light,

$$\begin{aligned} E &= hf = \frac{hc}{\lambda} = \frac{1243 \text{ eV nm}}{535 \text{ nm}} \\ &= 2.32 \text{ eV} \end{aligned}$$

For red light,

$$\begin{aligned} E &= hf = \frac{hc}{\lambda} = \frac{1243 \text{ eV nm}}{575 \text{ nm}} \\ &= 2.16 \text{ eV} \end{aligned}$$

Overall, it will be

$$\begin{aligned} E &= hf = \frac{hc}{\lambda} = \frac{1243 \text{ eV nm}}{555 \text{ nm}} \\ &= 2.23 \text{ eV} \end{aligned}$$

Similarly, photon energy for rod photoreceptor will be,

$$\begin{aligned} E &= hf = \frac{hc}{\lambda} = \frac{1243 \text{ eV nm}}{510 \text{ nm}} \\ &= 2.43 \text{ eV} \end{aligned}$$

(b)

$$\text{Light intensity} = 100 \mu\text{W/m}^2 = 100 \times 10^{-6} \text{ W/m}^2$$

$$E_{\text{photon}} = \frac{hc}{\lambda} = \frac{(6.63 \times 10^{-34}) \text{ J}\cdot\text{sec}(3 \times 10^8) \text{ m/sec}}{555 \times 10^{-9} \text{ m}} = 3.58 \times 10^{-19} \text{ J}$$

$$\text{Photon flux} = \frac{100 \times 10^{-6} \text{ W/m}^2}{3.58 \times 10^{-19} \text{ J}} = 2.8 \times 10^{14} \text{ photons/m}^2 \text{ sec}$$

(c)

$$\begin{aligned} \text{Number of cones} &= 150,000 / \text{mm}^2 = 1.5 \times 10^{11} / \text{m}^2 \\ \text{sensation time} &= \frac{1}{5} \text{ sec} = 0.2 \text{ sec} \end{aligned}$$

Number of photons required to excite the cone in 1 sec = 2.8×10^{14} photons/ m^2

Number of photons exciting the cones in 0.2 sec = $0.2 \times 2.8 \times 10^{14}$ photons/ m^2

One knows the areal density of cones, so the number of photons per cone will be,

$$= \frac{0.2 \times 2.8 \times 10^{14} \text{ photons/ m}^2}{1.5 \times 10^{11} / \text{m}^2} = 373 \text{ photons per cone}$$

(d)

For overall 10 percent efficiency of human eye,

number of photons absorbed per cone = $10 \times 373 = 3730$ photons per cone

Assignment 3: Wavelike properties of particles

1. In a diffraction experiment in which electrons of kinetic energy 110 eV are scattered from a crystal, a first maximum in the intensity of the scattered electrons occurs at an angle $\theta = 10.7^\circ$. (a) How many peaks will be there in the interference pattern? (b) What is the spacing between the crystal planes?
2. Thermal neutrons incident on a sodium chloride crystal (interatomic spacing 2.81 Å) undergo first order diffraction from the principle Bragg planes at an angle of 20° . What is the energy of the thermal neutrons? What is their temperature? (Use the principle of equipartition of energy treating the neutrons as point particles. The mass of a neutron is 1.67×10^{-27} kg.)
3. Calculate the kinetic energy of a proton of wavelength 0.5 fm? Use relativistic expressions. The rest mass of a proton is 1.67×10^{-27} kg.
4. A measurement establishes the position of a proton with an accuracy of $\pm 1.00 \times 10^{-11}$ m. Find the uncertainty in the proton's position 1.00 sec later. Assume that the speed of the proton $v \ll c$. Does the uncertainty increase or decrease with time?
5. An excited electron in an Na atom emits radiation at a wavelength 589 nm and returns to the ground state. If the mean time for the transition is about 20 ns, calculate the natural width of the emission line. What the "length" of the photon wavepacket?
6. Find the uncertainty in the location of a particle, in terms of its de Broglie wavelength λ , so that the uncertainty in its velocity is equal to its velocity.
7. Suppose at $t = 0$, a system is in a state given by the wavefunction,

$$\begin{aligned}\psi(x, 0) &= \frac{1}{\sqrt{a}} & |x| < a/2 \\ &= 0 & \text{otherwise.}\end{aligned}$$

If, at the same instant, the momentum of the particle is measured, what are the possible values that can be found and with what probability? One may like to use

these results for the Fourier transformation between momentum and real spaces.

$$\psi(x, 0) = \int A(k) e^{ikx} dk$$
$$A(k) = \frac{1}{2\pi} \int \psi(x, 0) e^{-ikx} dx.$$

8. The momentum of a particle is precisely measured at $\hbar k_0$. This means the wavepacket in momentum space is given by the delta function,

$$A(k) = \delta(k - k_0).$$

What is the wavefunction in real space and how large is the position uncertainty?

9. Special relativity tells us that no material particle can travel faster than light. Consider an electron with relativistic energy $E = mc^2$, m being the relativistic mass. The energy can also be expressed in terms of the relativistic momentum p and the rest mass, $E^2 = (m_0c^2)^2 + (pc)^2$. Find the phase and group velocities of the electron. You will notice that under some conditions, the phase velocity can exceed the speed of light. How do you resolve this paradox?
10. Why do electron microscopes have a higher resolution than optical microscopes?
11. A harmonic oscillator has energy,

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2, \quad (1)$$

where ω is the frequency of the oscillator. Classically $x = 0$, $p = 0$ results in a minimum energy equal to zero. Now use the uncertainty principle to estimate the minimum energy. Assume $\Delta p \sim p$ and $\Delta x \sim x$.

Wavelike properties of particles

Answer 1.

(a)

Start with the expression that tells you where maxima in scattering occur,

$$n\lambda = 2d \sin \theta .$$

Knowing that $\sin \theta_n = 0.18$ for $n = 1$, we want to find the value of d . Rewriting the above equation as,

$$d = \frac{\lambda}{2 \sin \theta_1} = \frac{\lambda}{2 \times 0.18} .$$

Thus to find the separation (d) we need the wavelength of electron, which we can find out by using the expression,

$$K = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} ,$$

where K is the kinetic energy of the electron. Therefore,

$$\lambda^2 = \frac{h^2}{2mK} = \frac{(6.63 \times 10^{-34} \text{ Js})^2}{2 (0.91 \times 10^{-30} \text{ Kg})(110 \text{ eV})(1.6 \times 10^{-19} \text{ J/eV})} = 1.37 \times 10^{-20} \text{ m}^2$$
$$\lambda = 1.17 \times 10^{-10} \text{ m} .$$

In turn, this gives,

$$d = \frac{1.17 \times 10^{-10} \text{ m}}{2 \times 0.186} = 3.14 \times 10^{-10} \text{ m} .$$

This will be the spacing between the crystal planes.

(b)

In the given problem, knowing the location of the first peak, we want to count the total number of peaks. The above equation can be written as,

$$\frac{n\lambda}{2d} = \sin \theta_n$$

As,

$$\begin{aligned}\sin \theta_n &\leq 1 \\ n \lambda &\leq 2 d \\ n &\leq \frac{2 d}{\lambda}\end{aligned}$$

Substituting values yields,

$$\begin{aligned}n &\leq \frac{2 \times 3.14 \times 10^{-10}}{1.17 \times 10^{-10}} \\ n &\leq 5.4\end{aligned}$$

We will see at the most 5 diffraction maxima.

Answer 2.

Given is the interatomic spacing $d = 2.81 \text{ \AA}$, $n = 1$, $\theta = 20^\circ$. We have to find the energy of thermal neutrons. For a first order Bragg's reflection,

$$\begin{aligned}n \lambda &= 2 d \sin \theta \\ \lambda &= 2 (2.81 \text{ \AA}) \sin 20^\circ \\ \lambda &= 2 (2.81 \text{ \AA}) (0.342) \\ \lambda &= 1.92 \text{ \AA}.\end{aligned}$$

Using the De Broglie's relation,

$$\begin{aligned}\lambda &= \frac{h}{p} \\ p &= \frac{h}{\lambda} \\ &= \frac{6.63 \times 10^{-34} \text{ J}\cdot\text{sec}}{1.92 \times 10^{-10} \text{ m}} \\ p &= 3.45 \times 10^{-24} \text{ Kg m/sec}.\end{aligned}$$

Kinetic energy will be calculated using the non-relativistic expression,

$$\begin{aligned}K &= \frac{p^2}{2m} = \frac{(3.45 \times 10^{-24} \text{ Kg m/sec})^2}{2 \times 1.67 \times 10^{-27} \text{ Kg}} \\ K &= 3.57 \times 10^{-21} \text{ J}.\end{aligned}$$

(b)

If we treat the neutrons as point particles, this means that the neutrons have only kinetic

energy and no potential energy. Since the neutrons can move in three orthogonal directions (x, y and z), there are three degrees of freedom. This means that the average kinetic energy is,

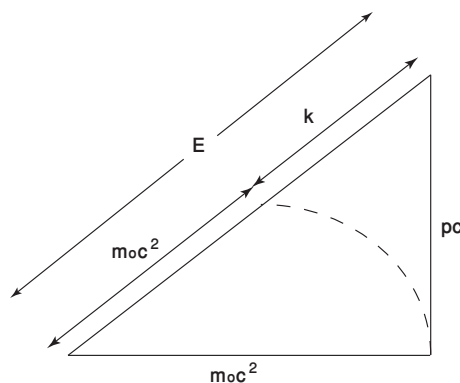
$$\begin{aligned}K &= 3 \times \frac{1}{2} k_B T = \frac{3}{2} k_B T. \\T &= \frac{2K}{3k_B} \\&= \frac{2 \times 3.57 \times 10^{-21} \text{ J}}{3 \times 1.38 \times 10^{-23} \text{ J/K}} \\T &= 172 \text{ K}.\end{aligned}$$

This is the approximate temperature of the thermal neutrons.

Answer 3

The De Broglie wavelength λ of a matter wave is given by,

$$\begin{aligned}\lambda &= \frac{h}{p} = \frac{hc}{pc} \\pc &= \frac{hc}{\lambda} = \frac{1243 \text{ eV nm}}{0.5 \times 10^{-15} \text{ m}} \\pc &\approx 2480 \text{ MeV}.\end{aligned}$$



Using the relativistic energy momentum relationship,

$$\begin{aligned}E^2 &= (pc)^2 + (m_0c^2)^2 \\&= (2480 \text{ MeV})^2 + (938 \text{ MeV})^2 \\E &\approx 2660 \text{ MeV}.\end{aligned}$$

Since the total energy is the sum of kinetic and rest-mass energy, therefore,

$$\begin{aligned} E &= K + E_o \\ K &= E - m_o c^2 \\ &= (2660 - 938) \text{ MeV} \\ &= 1720 \text{ MeV.} \end{aligned}$$

Answer 4

At time $t = 0$, the uncertainty in proton's position is Δx_o , then the uncertainty in the momentum will be,

$$\Delta p \geq \frac{\hbar}{2 \Delta x_o}.$$

Since $v \ll c$, then momentum uncertainty is,

$$\begin{aligned} \Delta p &= \Delta(mv) \\ &= m \Delta v. \end{aligned}$$

Then the uncertainty in proton's velocity is,

$$\Delta v = \frac{\Delta p}{m} \geq \frac{\hbar}{2 m \Delta x_o}.$$

The distance x the proton covers in time t cannot be known more accurately than,

$$\Delta x = t \Delta v \geq \frac{\hbar t}{2 m \Delta x_o}.$$

Here Δx is inversely proportional to Δx_o , the more we know about the proton's position at time $t = 0$, the less we know about its later position at $t > 0$.

The value of Δx at time $t = 1.00$ sec is,

$$\begin{aligned} \Delta x &\geq \frac{(1.054 \times 10^{-34} \text{ J sec}) (1.0 \text{ sec})}{2 (1.67 \times 10^{-27} \text{ Kg}) (1 \times 10^{-11} \text{ m})} \\ &\geq 3.15 \times 10^3 \text{ m,} \end{aligned}$$

which is 3.15 Km!

The uncertainty increases with time. As time proceeds, the position of the particle becomes more imprecise.

Answer 5

Given is the wavelength of emitted radiation $\lambda = 589\text{nm}$. $\Delta t = 20 \times 10^{-9}$.

Using the Heisenburg's uncertainty principle,

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

Since $E = hf$ which means $\Delta E = h \Delta f$. But

$$\begin{aligned}c &= f \lambda \\f &= \frac{c}{\lambda} \\ \Delta f &= \frac{-c \Delta \lambda}{\lambda^2} \\ |\Delta E| &= h \frac{c \Delta \lambda}{\lambda^2}.\end{aligned}$$

Therefore, the whole expression becomes,

$$\begin{aligned}\frac{hc \Delta \lambda}{\lambda^2} \Delta t &\approx \frac{\hbar}{2} \\ \Delta \lambda &\approx \frac{\hbar \lambda^2}{2 hc \Delta t} \\ &\approx \frac{h}{2\pi} \frac{1}{2hc} \frac{\lambda^2}{\Delta t} \\ &\approx \frac{1}{4\pi c} \frac{\lambda^2}{\Delta t} \\ &\approx \frac{1}{4\pi (3 \times 10^8 \text{ m/sec})} \frac{(589 \times 10^{-9})^2 \text{ m}^2}{20 \times 10^{-9} \text{ sec}} \\ &\approx 4.60 \text{ fm}.\end{aligned}$$

To find out the length of photon, we use the expression,

$$\Delta p = \hbar \Delta k.$$

From uncertainty relation,

$$\begin{aligned}\Delta x \Delta p &\approx \frac{\hbar}{2} \\ \Delta x (\hbar \Delta k) &\approx \frac{\hbar}{2} \\ \Delta x &\approx \frac{1}{2\Delta k}.\end{aligned}$$

Δk can be evaluated by using the expression,

$$\begin{aligned}k &= \frac{2\pi}{\lambda} \\|\Delta k| &= \frac{2\pi}{\lambda^2} \Delta\lambda \\&= \frac{2\pi}{(589 \times 10^{-9})^2 \text{ m}^2} 4.60 \times 10^{-15} \text{ m} \\|\Delta k| &= 0.08 \text{ m}^{-1}.\end{aligned}$$

Therefore, the length of photon will be,

$$\begin{aligned}\Delta x &\approx \frac{1}{2\Delta k} \approx \frac{1}{2 \times 0.08 \text{ m}^{-1}} \\ \Delta x &\approx 6.25 \text{ m}.\end{aligned}$$

Answer 6

When the uncertainty in the velocity of a particle is equal to its velocity, i.e. $\Delta v = v$. This means that,

$$\Delta p = m \Delta v = m v = p$$

Therefore, the uncertainty in its position will be given by,

$$\Delta x \geq \frac{\hbar}{\Delta p} = \frac{\hbar}{p} = \frac{h}{2\pi p}.$$

The De Broglie wavelength is related to the momentum by,

$$\lambda = \frac{h}{p}.$$

Hence, the uncertainty in the position of the particle is,

$$\Delta x \geq \frac{\lambda}{2\pi}.$$

Answer 7

The wave function in real space $\psi(x, 0)$ is related to the wave function in momentum space

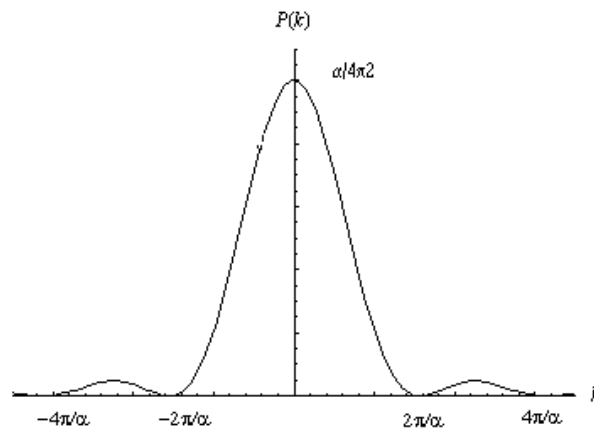
$A(k)$ through the given Fourier transform. Hence,

$$\begin{aligned}
 A(k) &= \frac{1}{2\pi} \int_{-a/2}^{a/2} \frac{1}{\sqrt{a}} e^{-ikx} dx \\
 &= \frac{1}{2\pi} \frac{1}{\sqrt{a}} \left. \frac{e^{-ikx}}{-ik} \right|_{-a/2}^{a/2} \\
 &= \frac{1}{-2\pi ik \sqrt{a}} \left(e^{-ika/2} - e^{ika/2} \right) \\
 &= \frac{1}{\pi k \sqrt{a}} \left(\frac{1}{2i} \right) \left(e^{-ika/2} - e^{ika/2} \right) \\
 &= \frac{1}{\pi k \sqrt{a}} \sin(ka/2)
 \end{aligned}$$

Now the probability of finding the wave number $k = p/\hbar$ is the modulus squared of $A(k)$.

$$\begin{aligned}
 |A(k)|^2 &= \frac{1}{\pi^2 k^2 a} \sin^2(ka/2) \\
 &= \frac{1}{\pi^2} \frac{a \sin^2(ka/2)}{4 k^2 a^2/4} \\
 &= \frac{a}{4\pi^2} \frac{\sin^2(ka/2)}{(ka/2)^2}
 \end{aligned}$$

The curve represents the probability of measuring the particle with momentum k . This



curve is called a sinc function. The most probable value of the momentum is zero.

Answer 8

The position wavefunction is,

$$\begin{aligned}\psi(x, 0) &= \int_{-\infty}^{\infty} \delta(k - k_o) e^{ikx} dk \\ &= e^{ik_o x}.\end{aligned}$$

We have used the property of the Dirac delta function.

$$\int_{-\infty}^{\infty} \delta(k - k_o) f(k) dk = f(k_o)$$

$\delta(k - k_o)$ is zero everywhere, except at $k = k_o$, where it is non-zero, and the area under it becomes unity. Therefore the integral vanishes everywhere except at $k = k_o$ and the integral equals the value of the function at $k = k_o$.

Now finding the probability,

$$|\psi(x, 0)|^2 = e^{-ik_o x} \cdot e^{ik_o x} = 1.$$

Hence the particle has a uniform probability of existing “anywhere“ in the space. The position uncertainty Δx is practically infinity.

Answer 9

The energy and momentum of a relativistic particle (in this case, electron) are given by,

$$E = m c^2 = \frac{m_o c^2}{\sqrt{1 - \frac{v^2}{c^2}}}. \quad (1)$$

$$p = m v = \frac{m_o v}{\sqrt{1 - \frac{v^2}{c^2}}}. \quad (2)$$

The energy in terms of the relativistic momentum p and the rest mass m_o can be obtained from the expression we have now encountered several times,

$$\begin{aligned}E^2 &= p^2 c^2 + m_o^2 c^4, \\ E &= c \sqrt{p^2 + m_o^2 c^2}.\end{aligned}$$

The corpuscular features (energy and momentum) of an electron are connected to its wave characteristics (wave frequency and number) by the relations,

$$E = \hbar \omega \quad \text{and} \quad p = \hbar k.$$

Therefore the group and phase velocities will become

$$v_g = \frac{d\omega}{dk} = \frac{dE}{dp}, \quad \text{and}$$

$$v_{ph} = \frac{E}{p} = \frac{E}{p}.$$

From Equation (1) and (2), we find that $p^2 + m_o^2 c^2 = \frac{m_o^2 c^2}{(1 - \frac{v^2}{c^2})}$. so, the phase velocity is

$$\begin{aligned} v_g &= \frac{dE}{dp} = \frac{d}{dp} \left(c \sqrt{p^2 + m_o^2 c^2} \right) \\ &= \frac{p c}{\sqrt{p^2 + m_o^2 c^2}} \\ &= \frac{m_o v c / \sqrt{1 - \frac{v^2}{c^2}}}{\frac{E}{c}} \\ &= \frac{m_o v c^2}{E \sqrt{1 - \frac{v^2}{c^2}}} \\ &= \frac{m_o v c^2}{\sqrt{1 - \frac{v^2}{c^2}}} \times \frac{\sqrt{1 - \frac{v^2}{c^2}}}{m_o c^2}. \end{aligned}$$

Hence $v_g = v$.

This shows that the speed of relativistic particle is equal to its group velocity.

Similarly, the phase velocity of relativistic particle can be calculated as

$$\begin{aligned} v_{ph} &= \frac{E}{p} \\ &= \frac{c \sqrt{p^2 + m_o^2 c^2}}{p} \\ &= c \sqrt{1 + \frac{m_o^2 c^2}{p^2}} \\ &= c \sqrt{1 + \frac{m_o^2 c^2}{m_o^2 v^2} \times \left(1 - \frac{v^2}{c^2}\right)} \\ &= c \sqrt{1 + \frac{c^2}{v^2} \left(1 - \frac{v^2}{c^2}\right)} \\ &= c \sqrt{\frac{c^2}{v^2}}. \end{aligned}$$

Hence $v_{ph} = c \left(\frac{c}{v} \right)$.

As $c > v$, this means $v_{ph} > c$, predicting that the phase velocity for the relativistic particle is greater than the speed of light c . This appears to be a violation of the postulates of special theory of relativity. Actually, the phase velocity does not represent the physical velocity of the particle, rather it is the group velocity which represents the speed of propagation of the particle.

Answer 10

The resolving power of an electron microscope is far better than that of an optical microscope because the wavelength associated with an electron is thousand times shorter than the wavelength of visible light. From the theory of single-slit diffraction, we know that spatial resolution $\delta\theta = \frac{\lambda}{d}$, where d is the diameter of the lens or the slit. If λ is small, spatial resolution $\delta\theta$ is small, so two closely spaced objects can be resolved. It is the wave nature of electrons which makes the electron microscope to show minor details, not visible with optical microscope.

Answer 11

The energy of harmonic oscillator is given by,

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2. \quad (3)$$

Here we assume that $\Delta p \sim p$ and $\Delta x \sim x$. Using the uncertainty principle,

$$\begin{aligned} \Delta p \Delta x &\geq \frac{\hbar}{2} \\ p = \Delta p &\approx \frac{\hbar}{2\Delta x} \approx \frac{\hbar}{2x}. \end{aligned}$$

Writing Equation (3) in terms of x ,

$$\begin{aligned} E &= \frac{\hbar^2}{4x^2 2m} + \frac{1}{2}m\omega^2x^2 \\ E &= \frac{\hbar^2}{8mx^2} + \frac{1}{2}m\omega^2x^2. \end{aligned}$$

To find out the minimum energy, we set $\partial E/\partial x = 0$, so,

$$\begin{aligned}\partial E/\partial x &= \frac{\hbar^2}{8m} \frac{\partial}{\partial x} \left(\frac{1}{x^2} \right) + \frac{1}{2} m\omega^2 \frac{\partial}{\partial x} (x^2) = 0 \\ &\frac{\hbar^2}{8m} \left(\frac{-2}{x} \right) + \frac{1}{2} m\omega^2 (2x) = 0 \\ &\frac{-\hbar^2}{4m x} + m\omega^2 x = 0 \\ m\omega^2 x &= \frac{\hbar^2}{4m x} \\ m\omega^2 x^2 &= \frac{\hbar^2}{4m} \\ x^2 &= \frac{\hbar^2}{4m^2\omega^2} \\ x &= \pm \sqrt{\frac{\hbar^2}{4m^2\omega^2}} \\ x &= \pm \frac{\hbar}{2m\omega} .\end{aligned}$$

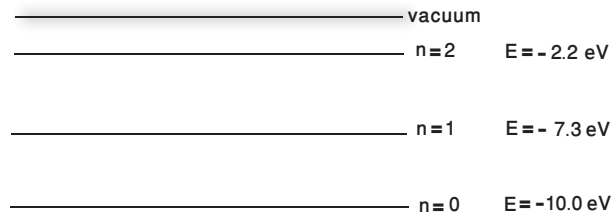
At this position, the energy of the harmonic oscillator will be minimum. If one tends to decrease x further, i.e., to squeeze the particle further, the energy shoots up again. To find the minimum, energy we substitute the expression in the above Equation (3),

$$\begin{aligned}E &= \frac{p^2}{2m} + \frac{1}{2} m\omega^2 \left(\frac{\hbar^2}{4m^2\omega^2} \right) \\ E &= \frac{p^2}{2m} + \frac{\hbar^2}{8m} .\end{aligned}$$

This is the required minimum energy of harmonic oscillator.

Assignment 4: Uncertainty principle, Bohr's model, Sommerfeld's quantization

1. The energy level diagram of an artificial atom is shown here.



- (a) Sketch the emission spectrum expected from a gas comprising of these artificial atoms. Identify the wavelengths.
- (b) In a real experiment, the spectral lines are observed to be broad rather than sharp. What are the possible causes of this broadening? Can the experimenter change his apparatus or experimental conditions to sharpen these lines?
- (c) What happens when a gamma ray photon strikes the atom?
- (d) The experimental spectrum indicates that the lines are not of the same brightness. Why is this so?
- (e) If the number of discrete levels is N , how many lines do you expect?
2. The ionization energy of hydrogen (^1H) is 13.6 eV. What is the ionization energy of tritium (^3H)?
3. A hydrogen atom in the ground state absorbs a 30.0 eV photon. What is the speed of the liberated electron? Is this speed quantized?
4. Consider a body rotating freely about a fixed axis. Apply the Wilson-Sommerfeld quantization rules, and show that the possible values of the total energy are predicted to be,
- $$E = \frac{n^2 \hbar^2}{2I} \quad n = 0, 1, 2, 3, \dots, \quad (1)$$
- where I is the moment of inertia.
5. What is the angular momentum of a photon emitted when an electron in a Bohr atom makes a transition from $n = 3$ to $n = 1$?

This description applies to the following questions.

As a consequence of the Heisenberg uncertainty principle the more closely an electron is confined to a region of space the higher its kinetic energy will be. In an atom the electrons are confined by the Coulomb potential of the nucleus. The competition between the confining nature of the potential and the liberating tendency of the uncertainty principle gives rise to various quantum mechanical effects. Some of these microscopic effects have repercussions in the way this universe is structured.

6. (a) Use the uncertainty principle to estimate the kinetic energy of an electron confined within a given radius r in a hydrogen atom. Assume that $\Delta p \sim p$ and $\Delta r \sim r$ (as in the previous assignment).
 - (b) Hence estimate the size of the hydrogen atom in its ground state by minimizing its total energy as a function of the orbital radius of the electron.
 - (c) Compare the size obtained in this way with the value obtained from a Bohr theory calculation.
-
7. When atoms are subjected to a high enough pressure they become ionized. This will happen, for example, at the center of a sufficiently massive gravitating body.
 - (a) In order to ionize an atom a certain minimum energy must be supplied to it, 13.6 eV, in the case of hydrogen. Estimate the reduction in atomic radius required to ionize a hydrogen atom.
 - (b) What pressure P is needed to bring this about? (Hint: $P = -\partial E/\partial V$ where E is energy and V is the volume.)
 - (c) A planet is defined as a body in which the atoms resist the compressive force of gravity. Estimate the maximum mass and size of a planet composed of hydrogen. (You will need to estimate the pressure required at the center of the planet to support a column of mass against its weight.)

This turns out to be of the order of the mass of Jupiter. Thus, Jupiter is not only the largest planet composed of hydrogen in the solar system but anywhere in the universe!

Uncertainty principle, Bohr's model, Sommerfeld's quantization

Answer 1.

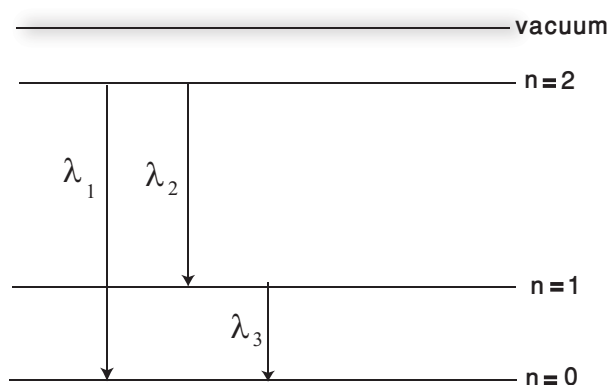
(a)

The emission of photons from the excited atoms will have specific wavelengths which corresponds to the energy difference between the higher and lower energy levels. In this particular case, the only discrete transitions that will occur are between the levels,

$$n = 2 \longrightarrow n = 0$$

$$n = 2 \longrightarrow n = 1$$

$$n = 1 \longrightarrow n = 0.$$



Hence the resulting spectrum will consist of three discrete spectral lines corresponding to the above mentioned transitions. We can identify the wavelengths by using the expression,

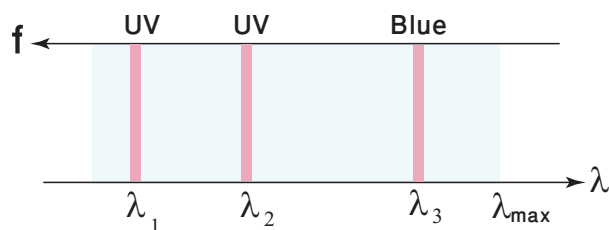
$$\begin{aligned} \Delta E &= hf \\ &= \frac{hc}{\lambda} \\ \lambda &= \frac{hc}{\Delta E}. \end{aligned}$$

Therefore, the wavelengths will be,

$$\begin{aligned}\lambda_1 &= \frac{hc}{E_2 - E_0} \\ &= \frac{1243 \text{ eV nm}}{-2.2 - (-10) \text{ eV}} \\ &= \frac{1243 \text{ eV nm}}{7.8 \text{ eV}} \\ \lambda_1 &= 159 \text{ nm (UV)}.\end{aligned}$$

$$\begin{aligned}\lambda_2 &= \frac{hc}{E_2 - E_1} \\ &= \frac{1243 \text{ eV nm}}{-2.2 - (-7.3)} \\ &= \frac{1243 \text{ eV nm}}{5.1 \text{ eV}} \\ \lambda_2 &= 243 \text{ nm (UV)}.\end{aligned}$$

$$\begin{aligned}\lambda_3 &= \frac{hc}{E_1 - E_0} \\ &= \frac{1243 \text{ eV nm}}{-7.3 - (-10)} \\ &= \frac{1243 \text{ eV nm}}{2.7 \text{ eV}} \\ \lambda_3 &= 460 \text{ nm (blue)}.\end{aligned}$$



Now, there will be a maximum wavelength which corresponds to the energy difference be-

tween vacuum and the immediate lower state ($n = 2$).

$$\begin{aligned} E &= (0 - (-2.2)) = hf \\ &= \frac{hc}{\lambda_{max}} \\ \lambda_{max} &= \frac{hc}{2.2 \text{ eV}} = \frac{1243 \text{ eV nm}}{2.2 \text{ eV}} \\ \lambda_{max} &= 565 \text{ nm} \end{aligned}$$

Below this particular value of the wavelength, the resulting spectrum will be continuous. A continuous spectrum is formed by electrons jumping from free space, which is a continuum, into one of the quantized levels. Therefore, the overall spectrum will be three discrete lines superposed on a continuous spectrum. The spectral lines and the continuous spectrum are indicated by pink and blue in the corresponding figure.

(b)

The spectral lines are observed to be broad rather than sharp because of several reasons. The first major factor which accounts for this observation is Doppler broadening. The thermal movement of atoms shifts the apparent frequency of each emitted photon. Since there is a distribution of speeds both towards and away from the observer in any gas sample, the net effect will be to broaden the observed line. For non-relativistic velocities, Doppler's shift in frequency is given by,

$$f = f_0 \left(1 \pm \frac{v}{c} \right),$$

where f_0 is the rest frequency, f is the observed frequency and v is the velocity of the atom with respect to the observer. This broadening mainly depends upon the frequency of the line and the temperature, pressure or density of the gas. As soon as we increase the temperature, the distribution of velocities becomes larger and consequently, the spectral lines broaden. One must cool the gas to make the lines sharper.

The second mechanism is called natural broadening and is a direct consequence of the uncertainty principle. The life time of electrons (average time they stay in excited states, Δt) is finite. The uncertainty relationship,

$$\Delta E \geq \frac{\hbar}{2\Delta t}$$

implies a spread in the energies or wavelengths. Clearly, this mechanism is not in the experimenter's control and is a manifestation of the fundamental dictates of the uncertainty

principle.

(c)

Gamma rays have wavelengths typically in the range of pico meter (pm) and consequently energies of the order of MeV. When they strike an atom, the electrons will absorb energy. Since the energy of incident photon is very high and the energy difference between $n = 0$ and vacuum is just 10 eV, therefore, gamma rays will always ionize the atom, freeing the electrons into vacuum.

(d)

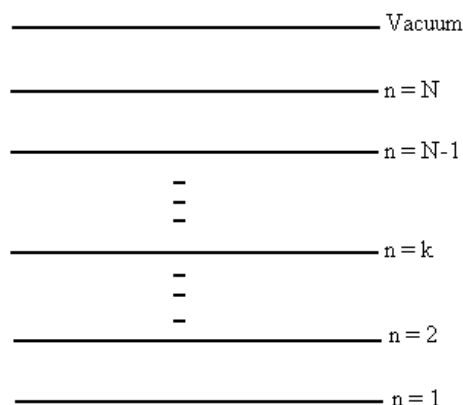
The brightness of the spectral lines depends upon the number of photons contributing to the emission lines. The number of photons emitted depends upon the number of electrons that jump from the higher to lower energy levels. However, all levels are not equally populated to start off with. The lower energy levels are more populated as compared to others. This can also be seen from Boltzmann's distribution, $P(E) = \frac{\exp(-E/kT)}{kT}$. Higher the energy of the level, lower will be the probability of finding electrons in that level. This uneven distribution of electrons results in lines of varying brightness.

(e)

The following table shows the relationship between the number of levels and the spectral lines for the smallest values of N .

No. of levels	spectral lines
2	1
3	3
4	6
5	10

One can also derive an exact formula for arbitrary N .



$$\begin{aligned}
 \text{Number of spectral lines} &= \sum_{k=1}^{N-1} (N - k) \\
 &= \sum_{k=1}^{N-1} N - \sum_{k=1}^{N-1} k \\
 &= N(N - 1) - \frac{(N - 1)}{2} \left(2(1) + ((N - 1) - 1)1 \right) \\
 &= N(N - 1) - \frac{(N - 1)}{2} (2 + N - 2) \\
 &= N(N - 1) - \frac{(N - 1)}{2} (N) \\
 &= (N - 1) \left(N - \frac{N}{2} \right) \\
 &= \frac{1}{2} N (N - 1).
 \end{aligned}$$

One can check the validity of this general result by plugging in the value of N and comparing it with the results presented in the Table.

Answer 2.

The Rydberg constant R_∞ assumes that the nucleus has infinite mass. For realistic atoms, this constant is corrected by using a reduced mass $\mu = m_e M / (m_e + M)$ for the electron, M being the mass of the nucleus. The corrected effective constant is then given by $R_\infty \mu / m_e$.

(The details are in Section 4.7 of the book.) Since the ionization energy is proportional to this constant, we get,

$$\frac{\text{ionization energy of hydrogen}}{\text{ionization energy of tritium}} = \frac{1 + \frac{m_e}{m_p + 2m_n}}{1 + \frac{m_e}{m_p}} \approx 0.9996,$$

indicating that the ionization energy of tritium is about 1.0004 times the ionization energy of normal hydrogen.

Answer 3

The energy of the incident photon is 30 eV. The energy of liberated electron will be equal to the difference between the incident photon energy and the ionization energy of hydrogen atom. Therefore, we can write the energy of liberated electrons as,

$$E = (30 - 13.6) \text{ eV} = \frac{1}{2} mv^2.$$

All of this energy appears as kinetic energy because the electron is free and has no potential energy. So,

$$\begin{aligned} v &= \sqrt{\frac{2(16.4) \text{ eV}}{m}} \\ &= \sqrt{\frac{2 (16.4) 1.6 \times 10^{-19} \text{ Kg m}^2/\text{s}^2}{9.11 \times 10^{-31} \text{ Kg}}} \\ &= \sqrt{5.76 \times 10^{12} \text{ m}^2/\text{sec}^2} \\ &= 2.4 \times 10^6 \text{ m/sec} . \end{aligned}$$

This speed will not be quantized because now, the electron is free, not bounded by the nucleus. Its energy can increase in arbitrarily small steps.

Answer 4

We know that Sommerfeld propose the quantization condition,

$$\oint p_q dq = nh ,$$

where p_q is the radial momentum canonically conjugate to the coordinate q and \oint represents integration over full orbital period. For a body rotating freely about a fixed axis, the angular momentum (L) will be canonically conjugate to the angular displacement (θ). Over

one complete period, θ varies from 0 to 2π helping us in fixing the limits of integration. Therefore,

$$\begin{aligned}\int_0^{2\pi} L d\theta &= nh \\ \int_0^{2\pi} I\omega d\theta &= nh \\ 2\pi I\omega &= nh \\ \omega &= \frac{nh}{2\pi I} \\ \omega &= \frac{n\hbar}{I},\end{aligned}$$

where I is the moment of inertia.

The total energy of the body will be,

$$\begin{aligned}E &= \frac{1}{2} I \omega^2 \\ &= \frac{1}{2} I \left(\frac{n\hbar}{I} \right)^2 \\ &= \frac{1}{2} I \frac{n^2 \hbar^2}{I^2} \\ E &= \frac{n^2 \hbar^2}{2I}. \quad n = 0, 1, 2, 3, \dots,\end{aligned}$$

These are the possible values of total energy. We see that the energy is quantized.

Answer 5

According to Bohr's quantization rule, the orbital angular momentum of an atomic electron moving under the influence of the Coulomb force is,

$$L = n\hbar.$$

When an electron in a Bohr atom makes a transition from $n = 3$ to $n = 1$, the change in angular momentum will be given by,

$$L = (3 - 1)\hbar = 2\hbar,$$

This is the momentum carried away by the photon. The particles whose angular momentum is an integral multiple of plank's constant \hbar are called bosons.

Answer 6

(a)

It is given that $\Delta p \sim p$ and $\Delta r \sim r$. When we consider small radii, the electron is present very close to the nucleus. Pushing the electron any closer to the nucleus results in increased energies. The electron may even gain enough energy to fly away from the nucleus. This is when the atom will ionize and hence the useful rule, "it is impossible to squish atoms". Close to the nucleus, we are "rubbing shoulders" with the uncertainty principle.

According to this principle, the momentum of an electron confined within a given radius r is approximately given by $p \sim \hbar/r$. (One could also use $p \sim \hbar/(2r)$ without affecting the overall implications of the result. Remember that the uncertainty principle is an *inequality!*) Therefore, when confined to a radius r , the kinetic energy will be of the order,

$$K.E = \frac{p^2}{2m} = \frac{\hbar^2}{2mr^2}.$$

Attempting to bring the nucleus any closer to the nucleus may result in extremely large kinetic energies, shooting the electron away.

(b)

In the closest approach of the electron to the nucleus, the total energy of the hydrogen atom is,

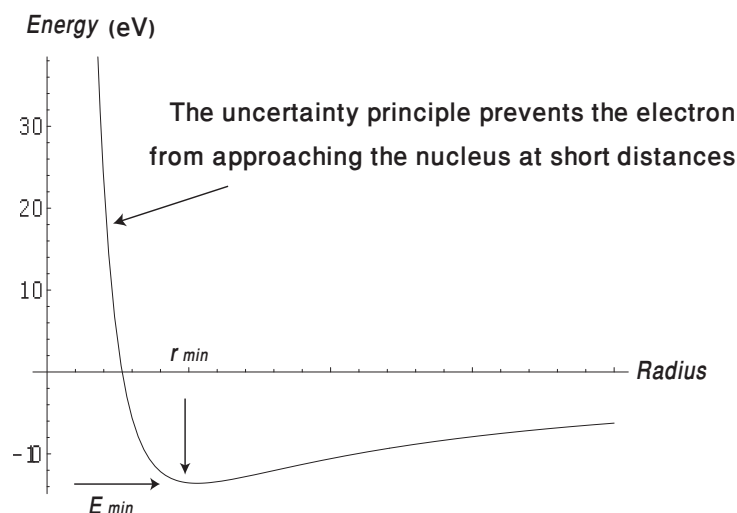
$$\begin{aligned} \text{Total Energy} &= E = K.E + P.E \\ &= \frac{\hbar^2}{2mr^2} - \frac{Ze^2}{4\pi\epsilon_0 r}. \end{aligned}$$

The energy is minimum when $dE/dr = 0$,

$$\begin{aligned} \frac{dE}{dr} &= \frac{\hbar^2}{2m} \frac{d}{dr} \left(\frac{1}{r^2} \right) - \frac{Ze^2}{4\pi\epsilon_0} \frac{d}{dr} \left(\frac{1}{r} \right) \\ &= \frac{\hbar^2}{2m} \left(\frac{-2}{r^3} \right) - \frac{Ze^2}{4\pi\epsilon_0} \left(\frac{-1}{r^2} \right) \\ &= \frac{-\hbar^2}{mr^3} + \frac{Ze^2}{4\pi\epsilon_0 r^2}. \end{aligned}$$

Setting this equal to zero,

$$\begin{aligned} \frac{-\hbar^2}{mr_{min}^3} + \frac{Ze^2}{4\pi\epsilon_0 r_{min}^2} &= 0 \\ \frac{Ze^2}{4\pi\epsilon_0 r_{min}^2} &= \frac{\hbar^2}{mr_{min}^3} \\ r_{min} &= \frac{4\pi\epsilon_0 \hbar^2}{mZe^2} \\ &= 0.53 \text{ \AA}, \end{aligned}$$



This is the radius, r_{min} , when the energy is minimum. The nucleus attracts the electron, so the electron prefers to exist close to the nucleus, but at the same time, the uncertainty principle does not let it come too close!

(c)

The value of the radius calculated above is in excellent agreement with the radius of the smallest orbit ($n = 1$) calculated from Bohr's model.

Answer 7

Using the information provided in Question 6: $\Delta p \sim p$ and $\Delta r \sim r$, and using the uncertainty principle, the momentum of an electron confined within a radius r is approximately $p \sim \hbar/r$. The total energy is,

$$\begin{aligned} \text{Total Energy} = E &= K.E + P.E \\ &= \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\epsilon_0 r}. \end{aligned}$$

Ionization occurs when the energy of the electron approached zero, the energy of the vacuum state. We calculate the radius r_{ion} when $E = 0$.

$$\begin{aligned} \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\epsilon_0 r} &= 0 \\ \frac{\hbar^2}{2mr^2} &= \frac{e^2}{4\pi\epsilon_0 r} \\ r_{ion} &= \frac{2\pi\epsilon_0 \hbar^2}{me^2} = 0.26 \text{ \AA}. \end{aligned}$$

The radius r_{ion} is smaller than the r_{min} calculated from the previous question, as we expect.

Excessive pressure inside a planet can push the electron to this radius. At this point, the atoms will ionize and the planet will not be stable.

(b)

The pressure is given as,

$$\begin{aligned} P &= -\frac{\partial E}{\partial V} \\ &= -\frac{\partial E}{\partial r} \frac{dr}{dV} \quad \text{using the chain rule.} \end{aligned}$$

Furthermore, we have,

$$\begin{aligned} V &= \frac{4}{3}\pi r^3 \\ dV &= 4\pi r^2 dr \\ \frac{dr}{dV} &= \frac{1}{4\pi r^2}. \end{aligned}$$

Differentiating the energy expression from (1),

$$\begin{aligned} \frac{\partial E}{\partial r} &= \frac{\hbar^2}{2m} \left(\frac{-2}{r^3} \right) - \frac{1}{4\pi\epsilon_0} e^2 \left(\frac{-1}{r^2} \right) \\ &= \frac{-\hbar^2}{mr^3} + \frac{e^2}{4\pi\epsilon_0 r^2}. \end{aligned}$$

We now substitute the value of the radius, $r = r_{ion}$,

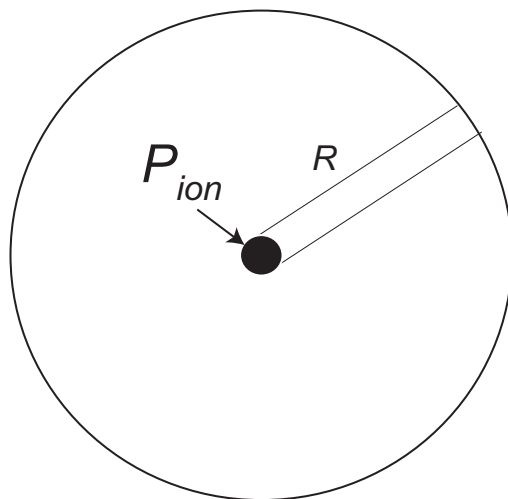
$$\left. \frac{\partial E}{\partial r} \right|_{r=r_{ion}} = \frac{-\hbar^2}{m} \left(\frac{1}{r_{ion}} \right)^3 + \frac{e^2}{4\pi\epsilon_0} \left(\frac{1}{r_{ion}} \right)^2 = -3.5 \times 10^{-7} \text{ J m}^{-1},$$

resulting in the ionizing pressure,

$$\begin{aligned} P_{ion} &= -\frac{\partial E}{\partial r} \frac{1}{4\pi r_{ion}^2} \\ &= 4.2 \times 10^{13} \text{ Pa.} \end{aligned}$$

(c)

We assume a spherical planet of radius R and mass M . We determine these parameters that result in ionizing pressures at the centre of the planet. First of all, we assume a constant density ρ of the planet throughout the interior. (You can appreciate that this is a very flaky assumption as one expects the density to be different in different parts of the planet, but



let's live with this assumption for the time being.) An estimate of the density is the proton mass divided by the volume of the atom,

$$\rho = \frac{m_p}{\frac{4}{3}\pi r_{ion}^3} = 2.3 \times 10^4 \text{ kg m}^{-3}. \quad (1)$$

The pressure exerted by a fluid of length R at its base is given by $\rho g R$. However, the value of g on this planet is unknown, but from Newton's law of gravitation, we know that $g = GM/R^2$. Therefore,

$$P_{ion} = \rho g R = \frac{\rho G M}{R} \quad (2)$$

$$\implies R = \frac{\rho G M}{P_{ion}} = 3.6 \times 10^{-20} M \text{ m}. \quad (3)$$

Now the density ρ can also be equated to the mass of the planet divided by its volume,

$$\rho = 2.3 \times 10^4 \text{ kg m}^{-3} = \frac{M}{\frac{4}{3}\pi R^3} \quad (4)$$

$$\implies M = \frac{4}{3}\pi \rho R^3. \quad (5)$$

Inserting the value of M into (3) and then back substituting results in,

$$M = 4.7 \times 10^{26} \text{ kg},$$

$$R = 1.7 \times 10^7 \text{ m}.$$

The measured mass and radius of Jupiter are $1.9 \times 10^{27} \text{ kg}$ and $7 \times 10^7 \text{ m}$ (values taken from Wikipedia).

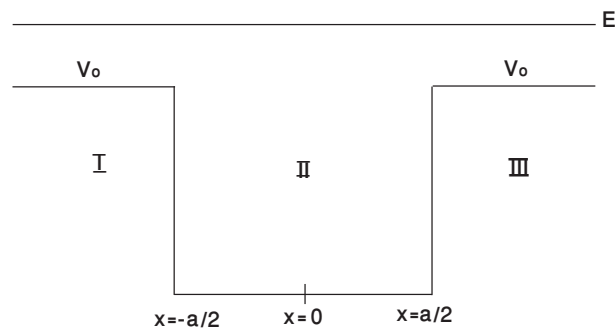
Assignment 5: Schrodinger wave equation and its applications

1. A particle of mass m , which moves freely inside an infinite potential well of length a , has the following initial wave function at $t = 0$,

$$\psi(x, 0) = \frac{A}{\sqrt{a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) + \sqrt{\frac{1}{5a}} \sin\left(\frac{5\pi x}{a}\right),$$

where A is a real constant.

- (a) Find A so that $\psi(x, 0)$ is normalized.
- (b) If measurements of the energy are carried out, what are the values that will be found and what are the corresponding probabilities? Calculate the average energy.
- (c) Are the measured energies equal to the average energy?
2. The wavefunction for a free electron, i.e., one on which no net force acts, is given by $\psi(x) = A \sin(2.5 \times 10^{10} x)$ where x is in meters. Compute the electron's (a) momentum, (b) de Broglie wavelength (c) total energy. (d) What is the uncertainty in the momentum?
3. Given is the following figure.

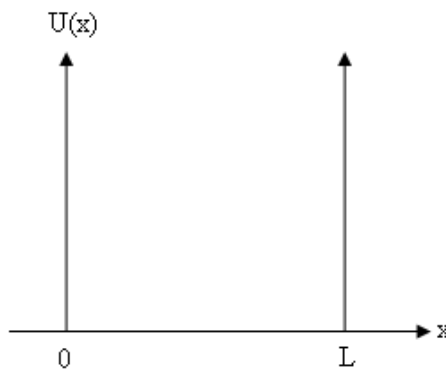


- A. Sketch an approximate wave function corresponding to the energy E .
- B. Is the energy quantized when $E > V_0$?
- C. What are the wave numbers in the regions I, II and III identified as $x < -a/2$, $-a/2 < x < a/2$, $x > a/2$ respectively?

For questions 4 – 7, consider an electron with the potential energy

$$U(x) = \begin{cases} 0 & 0 < x < L \\ \infty & x < 0 \text{ or } x > L \end{cases}$$

This potential energy function, plotted below, is often referred to as an infinite square well or a rigid box.



4. Suppose an electron with this potential energy function is in the state given by $\psi(x) = \frac{3}{5} \psi_1(x) + \frac{4}{5} \psi_2(x)$, where $\psi_1(x)$ and $\psi_2(x)$ are the two lowest energy states of this potential, with corresponding energies E_1 and E_2 . If you make a precise measurement of the energy of this electron, the result will be very close to which of the following values?
- A. At least $E_1 + E_2$
 - B. $(3/5) E_1 + (4/5) E_2$
 - C. $(3/5)^2 E_1 + (4/5)^2 E_2$
 - D. There is a $3/5$ probability of measuring E_1 and a $4/5$ probability of measuring E_2 .
 - E. There is a $9/25$ probability of measuring E_1 and a $16/25$ probability of measuring E_2 .
5. *After* the measurement described in the previous question, the energy of the *same electron* is precisely measured again. The result of this second measurement will be very close to which of the following values?

- A. The same value as in the first measurement.
 - B. Either E_1 or E_2 , with the relative probabilities of each being the same as for the first measurement, regardless of the result of the first measurement.
 - C. Either E_1 or E_2 , but the relative probabilities of each are not the same as they were for the first measurement.
 - D. If the second measurement occurs a very short time after the first measurement, statement A is correct, but if you wait a long time between the first and second measurement, statement B is correct.
 - E. None of the above statements are correct.
6. An electron with the same potential energy function (given above) is in the state $\psi(x) = \psi_1(x)$, so that its energy is E_1 . You measure the position of this electron, and the result of this measurement is that the position of the electron is $0.3L$. *After* this position measurement, you measure the *energy* of the same electron. Which of the following statements describes the result of this energy measurement?
- A. The value that you measure will definitely be E_1 .
 - B. The value that you measure could possibly be E_1 .
 - C. The value that you measure will definitely not be E_1 .
 - D. I have no idea how to answer this question.

Wavefunctions and Expectation Values

Answer 1.

(a)

A particle of mass m , moving freely inside an infinite potential well of length a , has the following wavefunction,

$$\psi(x, 0) = \frac{A}{\sqrt{a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) + \sqrt{\frac{1}{5a}} \sin\left(\frac{5\pi x}{a}\right).$$

Suppose that $\psi(x)$ is written as the superposition of three wavefunctions,

$$\psi(x) = \psi_1(x) + \psi_3(x) + \psi_5(x).$$

A measurement of position is performed. The measurement collapses $\psi(x)$ into either $\psi_1(x)$, $\psi_3(x)$ or $\psi_5(x)$ with certain probabilities. First we find out the normalization constant using the fact that the total probability of finding the particle in a well of length a is 1. Therefore,

$$\begin{aligned} P &= \int_{-a/2}^{a/2} \psi^*(x) \psi(x) dx = 1 \\ &= \int_{-a/2}^{a/2} \left(\frac{A}{\sqrt{a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) + \sqrt{\frac{1}{5a}} \sin\left(\frac{5\pi x}{a}\right) \right) \\ &\quad \left(\frac{A}{\sqrt{a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) + \sqrt{\frac{1}{5a}} \sin\left(\frac{5\pi x}{a}\right) \right) dx = 1 \\ &= \int_{-a/2}^{a/2} \left(\frac{A^2}{a} \sin^2\left(\frac{\pi x}{a}\right) + \frac{3}{5a} \sin^2\left(\frac{3\pi x}{a}\right) + \frac{1}{5a} \sin^2\left(\frac{5\pi x}{a}\right) + \right. \\ &\quad \left. \frac{A}{\sqrt{a}} \sqrt{\frac{3}{5a}} \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{3\pi x}{a}\right) + \dots \right) dx = 1. \end{aligned}$$

The integrand has 9 terms, 3 perfect squares and 6 mixed products. It is possible to show that the integral of each of the mixed products is zero. We explicitly show this only for one case, the $\sin(\pi x/a) \sin(3\pi x/a)$ term. We use the trigonometric relation,

$$\sin X \sin Y = \frac{1}{2}(\cos(X - Y) - \cos(X + Y)).$$

Therefore,

$$\begin{aligned}
 & \int_{-a/2}^{a/2} \left(\frac{A}{\sqrt{a}} \sqrt{\frac{3}{5a}} \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{3\pi x}{a}\right) \right) dx \\
 &= \frac{A}{2\sqrt{a}} \sqrt{\frac{3}{5a}} \int_{-a/2}^{a/2} \left(\cos\left(\frac{\pi x}{a} - \frac{3\pi x}{a}\right) - \cos\left(\frac{\pi x}{a} + \frac{3\pi x}{a}\right) \right) dx \\
 &= \frac{A}{2\sqrt{a}} \sqrt{\frac{3}{5a}} \int_{-a/2}^{a/2} \left(\cos\left(\frac{-2\pi x}{a}\right) - \cos\left(\frac{4\pi x}{a}\right) \right) dx \\
 &= \frac{A}{2\sqrt{a}} \sqrt{\frac{3}{5a}} \int_{-a/2}^{a/2} \left(\cos\left(\frac{2\pi x}{a}\right) - \cos\left(\frac{4\pi x}{a}\right) \right) dx \\
 &= \frac{A}{2\sqrt{a}} \sqrt{\frac{3}{5a}} \left(\frac{\sin\left(\frac{2\pi x}{a}\right)}{\frac{2\pi}{a}} - \frac{\sin\left(\frac{4\pi x}{a}\right)}{\frac{4\pi}{a}} \right) \Big|_{-a/2}^{a/2} \\
 &= \frac{A\sqrt{3}}{4\pi\sqrt{5}} \left(\sin\left(\frac{2\pi x}{a}\right) - \frac{1}{2} \sin\left(\frac{4\pi x}{a}\right) \right) \Big|_{-a/2}^{a/2} \\
 &= \frac{A\sqrt{3}}{4\pi\sqrt{5}} \left((\sin(\pi) + \sin(\pi)) - \frac{1}{2}(\sin 2\pi + \sin 2\pi) \right) \\
 &= 0.
 \end{aligned}$$

In this way, all the last six terms will be equal to zero, we left with,

$$\begin{aligned}
 & \int_{-a/2}^{a/2} \left(\frac{A^2}{a} \sin^2\left(\frac{\pi x}{a}\right) + \frac{3}{5a} \sin^2\left(\frac{3\pi x}{a}\right) + \frac{1}{5a} \sin^2\left(\frac{5\pi x}{a}\right) \right) dx = 1 \\
 & \int_{-a/2}^{a/2} \left(\frac{A^2}{a} \frac{1 - \cos\left(\frac{2\pi x}{a}\right)}{2} + \frac{3}{5a} \frac{1 - \cos\left(\frac{6\pi x}{a}\right)}{2} + \frac{1}{5a} \frac{1 - \cos\left(\frac{12\pi x}{a}\right)}{2} \right) dx = 1
 \end{aligned}$$

$$\frac{A^2}{a} \left(\frac{x}{2} - \frac{\sin\left(\frac{2\pi x}{a}\right)}{2 \frac{2\pi}{a}} \right) \Big|_{-a/2}^{a/2} + \frac{3}{5a} \left(\frac{x}{2} - \frac{\sin\left(\frac{6\pi x}{a}\right)}{2 \frac{6\pi}{a}} \right) \Big|_{-a/2}^{a/2} + \frac{1}{5a} \left(\frac{x}{2} - \frac{\sin\left(\frac{12\pi x}{a}\right)}{2 \frac{12\pi}{a}} \right) \Big|_{-a/2}^{a/2} = 1,$$

where $\sin\left(\frac{\pi x}{a}\right) \Big|_{-a/2}^{a/2} = 0$,

$$\begin{aligned}
 \frac{A^2}{a} \frac{2a}{4} + \frac{3}{5a} \frac{2a}{4} + \frac{1}{5a} \frac{2a}{4} &= 1 \\
 \frac{A^2}{2} + \frac{3}{10} + \frac{1}{10} &= 1 \\
 A^2 &= \frac{12}{10} \\
 A &= \sqrt{\frac{6}{5}},
 \end{aligned}$$

which is the required normalization constant. Hence the wavefunction in its normalized form is,

$$\psi(x, 0) = \sqrt{\frac{6}{5a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) + \sqrt{\frac{1}{5a}} \sin\left(\frac{5\pi x}{a}\right).$$

(b)

As the wavefunction collapses to one of the states, the corresponding eigen energies will be measured. In order to calculate the energy of each state, we use Schrodinger's equation

$$\frac{-\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x).$$

Since the particle is free, $V(x) = 0$, resulting in,

$$\frac{-\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x).$$

For collapse into $\psi_1(x)$, the measured energy will be E_1 .

$$\begin{aligned} \frac{-\hbar^2}{2m} \frac{d^2\psi_1(x)}{dx^2} &= E_1 \psi_1(x) \\ \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \left(\sqrt{\frac{6}{5a}} \sin\left(\frac{\pi x}{a}\right) \right) &= E_1 \psi_1(x) \\ \frac{-\hbar^2}{2m} \sqrt{\frac{6}{5a}} \frac{\pi}{a} \frac{d}{dx} \left(\cos\left(\frac{\pi x}{a}\right) \right) &= E_1 \psi_1(x) \\ \frac{+\hbar^2}{2m} \sqrt{\frac{6}{5a}} \frac{\pi^2}{a^2} \left(\sin\left(\frac{\pi x}{a}\right) \right) &= E_1 \psi_1(x) \\ \frac{\hbar^2 \pi^2}{2ma^2} \left(\sqrt{\frac{6}{5a}} \sin\left(\frac{\pi x}{a}\right) \right) &= E_1 \psi_1(x) \\ \frac{\hbar^2 \pi^2}{2ma^2} \psi_1(x) &= E_1 \psi_1(x). \end{aligned}$$

By comparison,

$$E_1 = \frac{\hbar^2 \pi^2}{2ma^2}.$$

Similarly for $\psi_3(x)$,

$$\begin{aligned} \frac{-\hbar^2}{2m} \frac{d^2\psi_3(x)}{dx^2} &= E_3 \psi_3(x) \\ \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \left(\sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) \right) &= E_3 \psi_3(x) \\ \frac{-\hbar^2}{2m} \sqrt{\frac{3}{5a}} \frac{3\pi}{a} \frac{d}{dx} \left(\cos\left(\frac{3\pi x}{a}\right) \right) &= E_3 \psi_3(x) \\ \frac{+\hbar^2}{2m} \sqrt{\frac{3}{5a}} \frac{9\pi^2}{a^2} \left(\sin\left(\frac{3\pi x}{a}\right) \right) &= E_3 \psi_3(x) \\ \frac{9\hbar^2 \pi^2}{2ma^2} \left(\sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) \right) &= E_3 \psi_3(x) \\ \frac{9\hbar^2 \pi^2}{2ma^2} \psi_3(x) &= E_3 \psi_3(x), \end{aligned}$$

resulting in,

$$E_3 = \frac{9\hbar^2 \pi^2}{2ma^2}.$$

Similarly, energy corresponding to the next state is,

$$E_5 = \frac{25\hbar^2 \pi^2}{2ma^2}.$$

If a measurement is carried out on the system, we would obtain either of these energies with the corresponding probability $P(E_n)$. Since the initially given wavefunction contains only three eigen states namely $\psi_1(x)$, $\psi_3(x)$ and $\psi_5(x)$, the possible energy measurements are,

$$\begin{aligned} E_1 &= \frac{\pi^2 \hbar^2}{2ma^2}, \\ E_3 &= \frac{9\pi^2 \hbar^2}{2ma^2}, \quad \text{and} \\ E_5 &= \frac{25\pi^2 \hbar^2}{2ma^2}, \end{aligned}$$

with the corresponding probabilities,

$$\begin{aligned} P_1(E_1) &= \int_{-a/2}^{a/2} \psi_1^*(x) \psi_1(x) dx = \frac{3}{5} \\ P_3(E_3) &= \int_{-a/2}^{a/2} \psi_2^*(x) \psi_2(x) dx = \frac{3}{10} \\ P_5(E_5) &= \int_{-a/2}^{a/2} \psi_3^*(x) \psi_3(x) dx = \frac{1}{10}. \end{aligned}$$

The average or expectation value of the energy will be equal to,

$$\begin{aligned}\langle E \rangle = E_{avg} &= \sum_n P(E_n) = P_1 E_1 + P_3 E_3 + P_5 E_5 \\ &= \frac{3}{5} E_1 + \frac{3}{10} E_3 + \frac{1}{10} E_5 \\ E_{avg} &= \frac{29\pi^2 \hbar^2}{10ma^2}.\end{aligned}$$

(c)

The expectation or average value of the energy is not equal to any of the measured values. This is very similar to the throws of a dice. The average value is 3.5 but this is never an outcome of a single throw! **Answer 2.**

The wavefunction of a free electron is given by,

$$\psi(x) = A \sin(2.5 \times 10^{10} x).$$

Since x is in meters, the constant 2.5×10^{10} must have the dimensions of m^{-1} to keep the argument of the *sin* function dimensionless. To calculate the required quantities, we start with the time-independent Schrodinger equation,

$$\frac{-\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x).$$

Since the particle is free, $V(x) = 0$, leading to the simpler form,

$$\frac{-\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x). \tag{1}$$

Making use of the given wavefunction, we obtain,

$$\begin{aligned}\frac{d^2\psi(x)}{dx^2} &= \frac{d}{dx} \left(\frac{d}{dx} (A \sin(2.5 \times 10^{10} x)) \right) \\ &= (2.5 \times 10^{10}) \frac{d}{dx} (A \cos(2.5 \times 10^{10} x)) \\ &= -(2.5 \times 10^{10})(2.5 \times 10^{10}) A \sin(2.5 \times 10^{10} x) \\ \frac{d^2\psi(x)}{dx^2} &= -(2.5 \times 10^{10})^2 \psi(x),\end{aligned}$$

and the R.H.S becomes,

$$\frac{-\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = \frac{\hbar^2}{2m} (2.5 \times 10^{10})^2 \psi(x),$$

comparing with the R.H.S of expression (1), we obtain,

$$\frac{\hbar^2}{2m} (2.5 \times 10^{10})^2 \psi(x) = E \psi(x)$$
$$E = \frac{(2.5 \times 10^{10})^2 \hbar^2}{2m},$$

which is the required energy of the free electron. In case of the free particle, the total energy is just equal to the kinetic energy and contribution of the potential energy is zero.

(a)

To compute the momentum of free electron, we use,

$$\text{Total Energy} = E = K.E = \frac{p^2}{2m}$$
$$p^2 = 2mE$$
$$p = \pm\sqrt{2mE}$$
$$= \pm\sqrt{2m \frac{(2.5 \times 10^{10})^2 \hbar^2}{2m}}$$
$$= \pm(2.5 \times 10^{10}) \hbar \quad (\text{Kg m s}^{-1}).$$

This is the momentum of the free electron.

(b)

The wavelength of the free electron is,

$$\lambda = \frac{h}{p} = \frac{h}{(2.5 \times 10^{10}) \frac{h}{2\pi}} = \frac{2\pi}{(2.5 \times 10^{10})} = 2.5 \times 10^{-10} = 2.5 \text{ \AA}.$$

(c)

As we have find out the exact value of momentum, therefore the uncertainty in momentum is zero ($\Delta p = 0$). On the other hand, uncertainty in position will be infinite ($\Delta x = \infty$).

Answer 3.

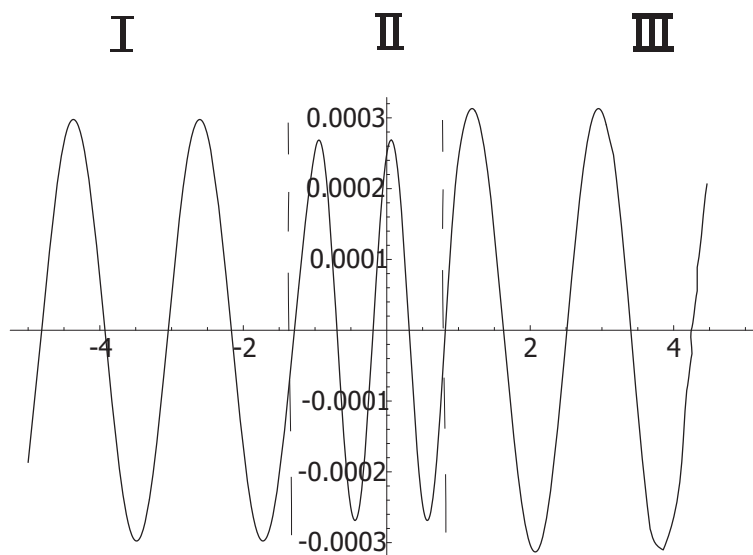
(a)

For the problem of the finite square well potential, when the total energy is greater than the potential energy, ($E > V_o$), the wavefunction will display an oscillating pattern. This can be seen from the Schrodinger equation,

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2} (V - E_o) \psi.$$

This equation show that $\psi(x)$ will be concave downwards when ψ is positive and concave upwards when ψ is negative. The bending is sharper when $|V - E_o|$ is larger; this is the

region labeled II. In regions I and III, the bending is gentler, the maximum amplitude is higher and the separation between the nodes is also larger.



It is also clear from the figure that the behavior of wavefunction is symmetric about $x = 0$ and identical in regions I and III.

(b)

The energy will not be quantized because the particle is not confined and is free to move in any direction. The energy is only quantized when the particle is confined within some region and its energy is less than the barrier potential ($E < V_o$).

(c)

Solving equation (1), the wavefunction is

$$\psi(x) = A \exp(ikx) + B \exp(-ikx).$$

The value of the potential is non zero in region I ($x < -a/2$) and III ($x > a/2$), so the wave numbers in these two regions will be,

$$k = \frac{\sqrt{2m(E - V_o)}}{\hbar}.$$

In region II, the wavenumber will be,

$$k = \frac{\sqrt{2mE}}{\hbar}.$$

Answer 4.

(a) E

When an electron is in the superposition of two or more wavefunctions and you make a measurement of the energy of this electron, then the wavefunction collapses into an energy eigenstate. The probability of finding energy E_1 will be simply equal to modulus squared of the amplitude accompanying $\psi_1(x)$. So, the probability of obtaining the value E_1 is $9/25$ and the probability of obtaining the value E_2 is $16/25$.

(b) A

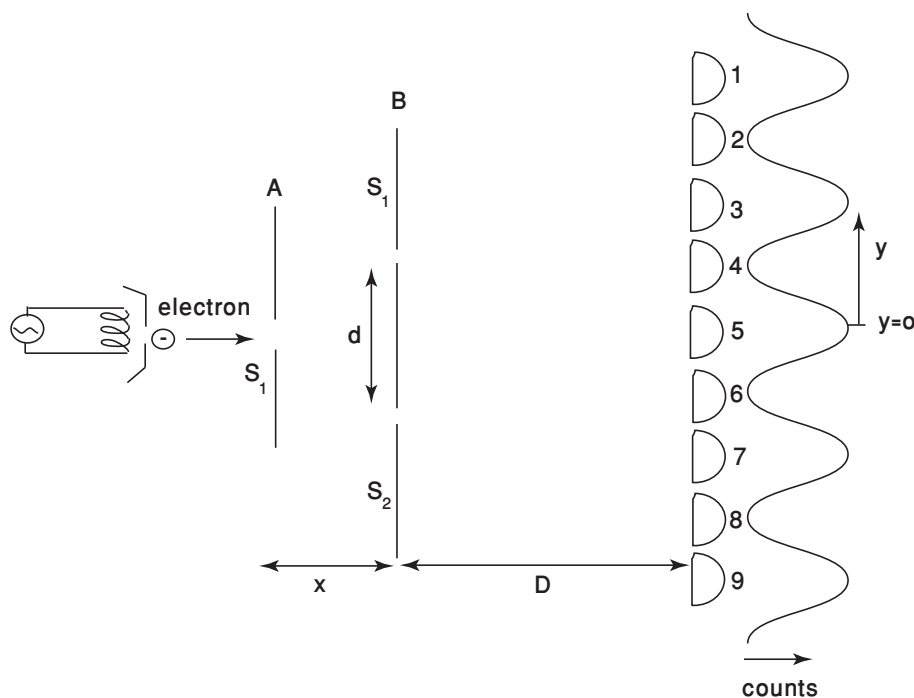
After the first measurement, you are again interested in measuring the energy of the same electron. Since the wavefunction is already collapsed and the state becomes an eigen state of energy, the consecutive measurement will yield same value of energy as in the first case, (with probability one).

(b) A

Since position and energy are not conjugate variables, therefore, the result of measuring the position of the electron will not effect the energy of that electron. After precisely measuring the position, if you measure the energy again, you will get the same value of energy.

Midterm Examination: Modern Physics

Consider an experiment in which an electron source is placed in front of screens A and B . A has a narrow slit S_1 , B has two slits S_1 and S_2 . Detectors are placed at a distance D from B , and are numbered from 1 to N . The clicks registered by each detector are counted and at the end of the day-long experiment the counts are plotted.



The pattern of the counts is shown in the rightmost part of the diagram. The detectors are coincident with the maxima and the minima of the fringes. The source emits only one electron at a time and the time between consecutive electron emissions $\Delta t > (D + x)/c$, where c is the speed of light. Now answer the following questions.

1. Which of the following statements is true? (3 Marks)
 - A. At one instant, all odd numbered detectors click together.
 - B. At one instant, all even numbered detectors click together.
 - C. More than one detector click at a time.
 - D. At one instant, only one of the odd-numbered detectors clicks.

E. None of the above are correct.

2. The fringes shown to the right of the detector array represent: (3 Marks)

A. The electric field of a single electron.

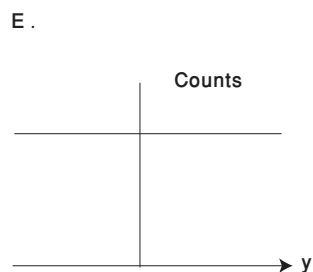
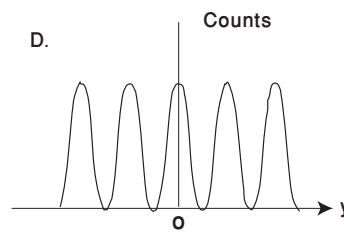
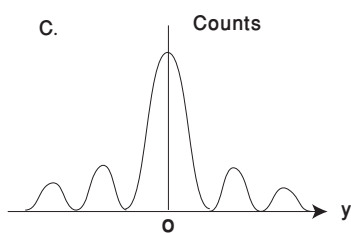
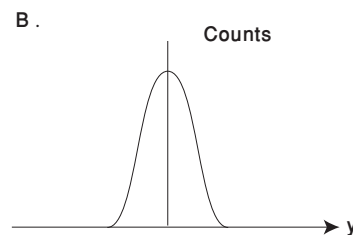
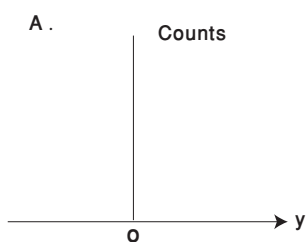
B. The momentum of a large number of electrons.

C. The wavefunction of a single electron $\psi(y)$.

D. The probability of the detectors clicking as a single electron traverses the apparatus.

E. The probability of the detectors clicking *after* many electrons have traveled through the apparatus.

3. If the screen B is completely removed, what form of the distribution of counts would you expect? (3 Marks)



4. The visibility of the fringes is defined as:

$$\frac{C_{max} - C_{min}}{C_{max} + C_{min}}$$

where C_{max} is the maximum number of counts registered by any detector and C_{min} is the minimum number of counts. In this way, the visibility represents the contrast of the fringes. Now, if the experiment is allowed to run for 12 hours instead of 24 hours, what will happen to the visibility of the fringes? (3 Marks)

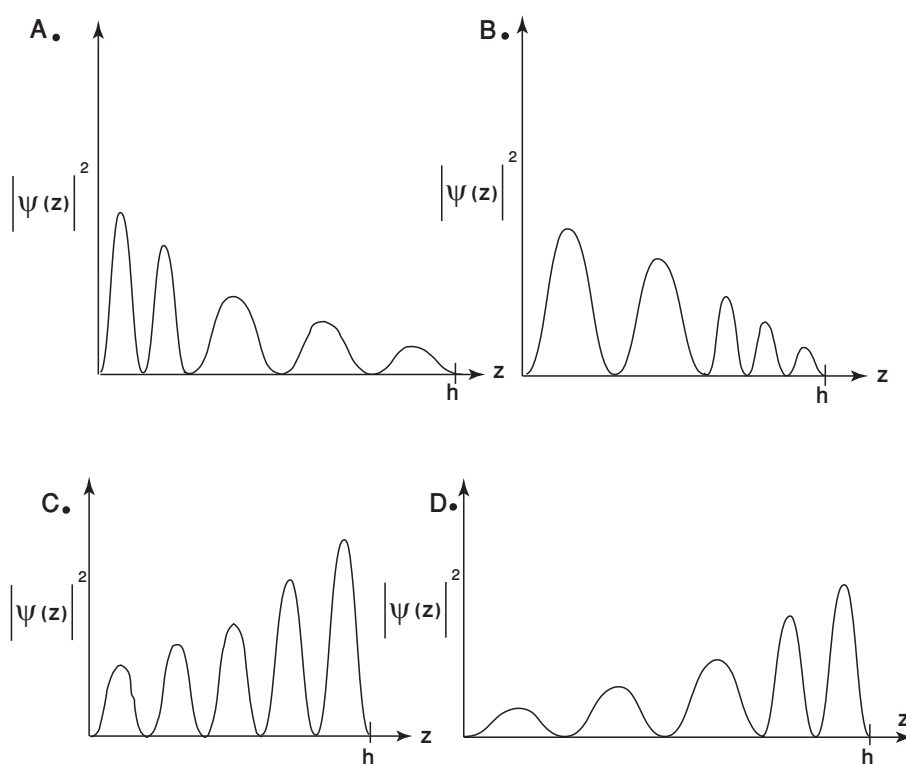
- A. It will have no effect as the fringes are formed by the interference of a single electron.
 - B. The visibility will double as we are now measuring for only half the time, and decreasing the time for which we disturb the system.
 - C. The visibility will halve.
 - D. We will not see any interference pattern at all.
 - E. None of the above.
5. The electrons are now replaced by neutrons moving with the same speed. How does the spacing between the maxima in the interference pattern change? (3 Marks)
- A. The spacing increases.
 - B. The spacing decreases.
 - C. The spacing remains unchanged
 - D. The fringes will disappear altogether because the neutrons do not carry an electric charge.
 - E. None of the above.
6. An adventurous experimenter sets out to demonstrate interference for C_{60} molecules. His experiment is undoubtedly more difficult than electrons. He will have a better chance of observing interference fringes: (5 Marks)
- A. By increasing the inter-slit distance d .
 - B. By decreasing both the distances d and D .

C. By increasing the ratio D/d .

D. By increasing the velocity of the C_{60} molecules.

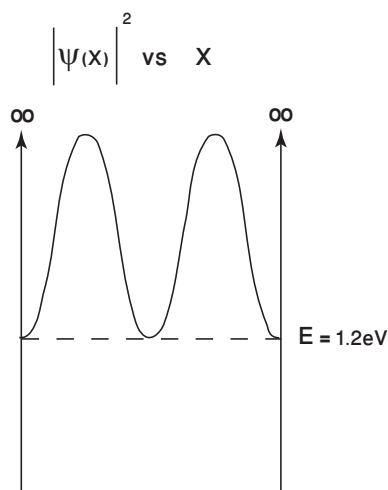
E. By allowing only one C_{60} molecule to pass through the apparatus.

7. In an experiment, a calcium ion Ca^{2+} is dropped from a height h . It falls under the action of gravity and rebounds from a flat surface (at $z = 0$) back up to the same height. There is no loss of energy anywhere. Which of these plots would be the best representation of the probability density $|\psi(z)|^2$ versus z , of a particular eigenstate of the system? (5 Marks)



E. None of the above.

8. A particle is in an infinite potential well. It is in an eigenstate such that its probability density $|\psi(x)|^2$ versus x is shown here.



The energy of the state is 1.2 eV. What is the energy of the lowest possible allowed energy state in this well? (3 Marks)

- A. 0.0 eV
- B. 0.3 eV
- C. 0.6 eV
- D. 1.2 eV
- E. We cannot be certain of the lowest energy state.

9. The position wavefunction, $\psi(x)$ of a particle at some instant is given by,

$$\psi(x) = \frac{1}{L^2 + (x - x_o)^2/\alpha^2},$$

where L, x_o, α are constants. Which of the following expression below is a good approximate to the spread in the momentum, Δp ? (5 Marks)

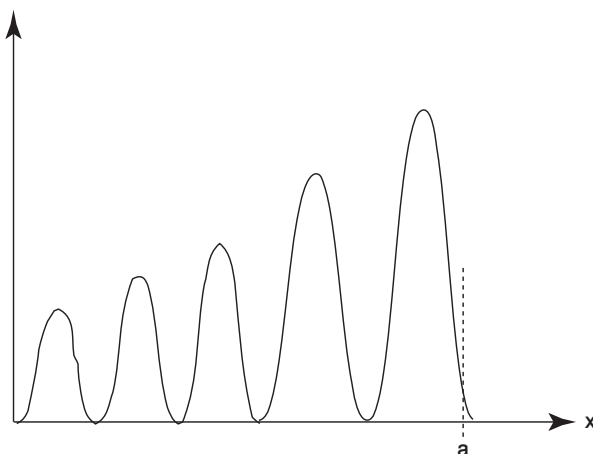
- A. $\Delta p \sim \hbar/(\alpha L)$
- B. $\Delta p \sim \hbar/\alpha$

C. $\Delta p \sim \hbar/(\alpha^2 x_o)$

D. $\Delta p \sim \hbar/(\alpha^2 L^2)$

E. $\Delta p \sim \hbar/(\alpha x_o)$

10. The probability density of a particle of energy E is shown in the diagram.



The particle is trapped inside a triangular potential well. Which of the following is the most likely form of the potential well? **See the next page for the potentials.**
(5 Marks)

11. The somewhat artificial wavefunction of a particle $\psi(x)$ is shown in the figure (**on page 8**). (Ignore the continuity requirement of the wavefunction.) The wavefunction is zero elsewhere. An experiment aims at measuring the position of many such particles. What is the spread Δx in the position measurements? (10 Marks)
12. Two ultraviolet and blue-violet beams of wavelengths 280 nm and 490 nm fall on a lead surface, they produce photoelectrons with maximum energies 8.57 eV and 6.67 eV, respectively. Using this data, estimate the numerical value of the Planck constant. (5 Marks)
13. A photon of energy hf strikes a proton of mass m_p . The Compton shift in wavelength is given by $\Delta\lambda = (h/(m_p c)) (1 - \cos\theta)$, where θ is the angle at which the photon is scattered. What is the maximum kinetic energy that can be transferred to the proton? (10 Marks)

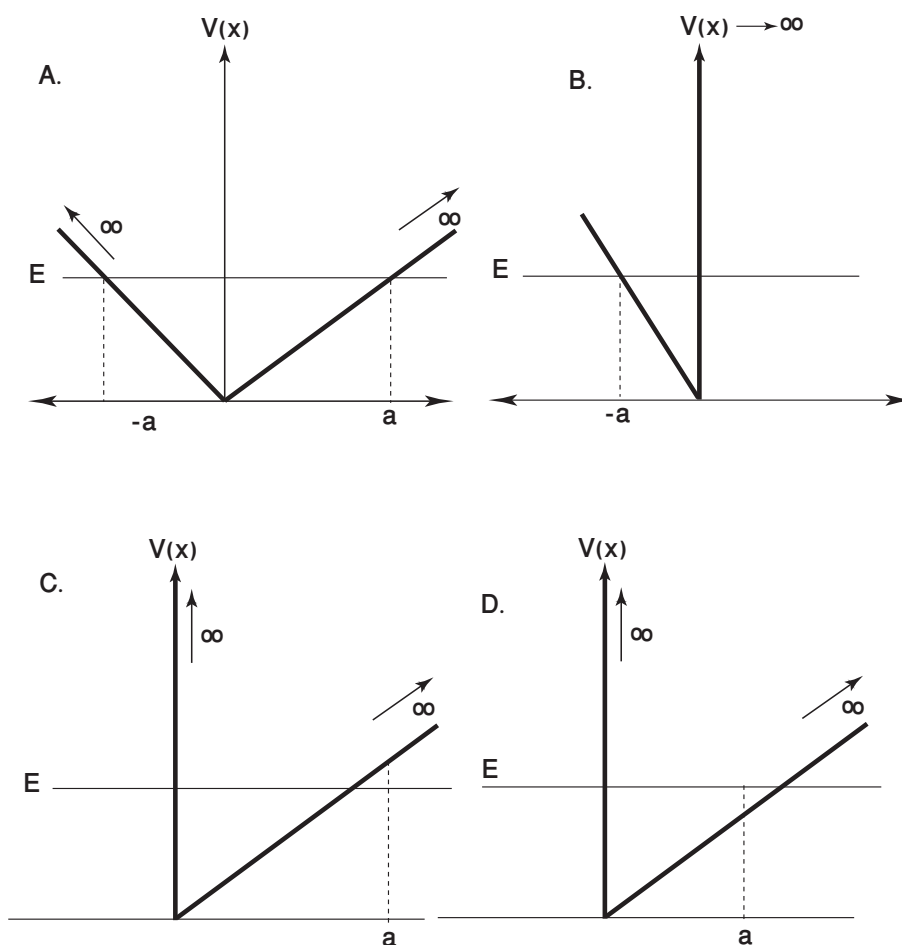


FIG. 1: Figure for Q. 10.

14. One wishes to measure the kinetic energy of an electron whose speed is 10.0 m/sec with an uncertainty of no more than 0.1%.

- How much time is needed to make this measurement?
- How far will the electron have traveled this period of time?

(10 Marks)

15. In this question, we will use some of the principles underlying Bohr's model. Two quarks have identical mass m and are revolving around one another.

- Assume that one of the quarks is fixed in space. What is the reduced mass μ of the revolving quark?

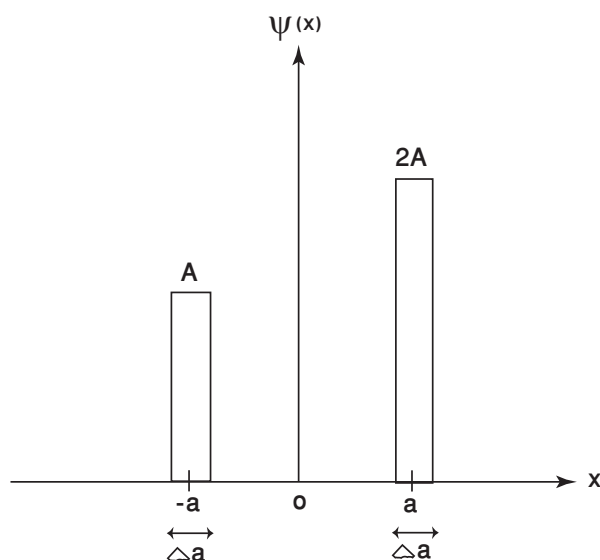


FIG. 2: Figure for Q 11.

- (b) The distance between the quarks is r , and the centripetal force $F = \mu v^2/r$ is assumed to be a constant. Using the quantization of angular momentum, calculate the radius of the smallest orbit.
- (c) If the radius of the first orbit is r_o , what is the radius of the second orbit? Is the radius quantized?
- (d) Calculate the quantized total energy and its dependence on the quantum number.
- (15 Marks)

Mid term solutions

Answer 1. D

Answer 2. D

Answer 3. C

Answer 4. C

Answer 5. B

Answer 6. C

Answer 7. C or E

Answer 8. B

Answer 9. A

Answer 10. C

Answer 11.

First we will normalize the given wave-function. From the given figure, we can write the

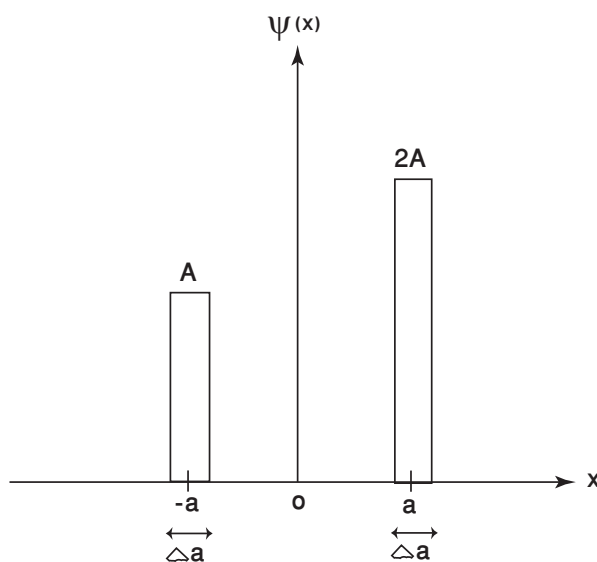


FIG. 1: Figure for Q 11.

wavefunction as,

$$\psi(x) = \begin{cases} A & -a - \frac{\Delta a}{2} < x < -a + \frac{\Delta a}{2} \\ 2A & a - \frac{\Delta a}{2} < x < a + \frac{\Delta a}{2} \end{cases}$$

Using the normalization condition, we first need to find out the normalization constant, A ,

$$\begin{aligned} \int_{-a-\Delta a/2}^{-a+\Delta a/2} A^2 dx + \int_{a-\Delta a/2}^{a+\Delta a/2} (2A)^2 dx &= 1 \\ A^2 x \Big|_{-a-\Delta a/2}^{-a+\Delta a/2} + 4A^2 x \Big|_{a-\Delta a/2}^{a+\Delta a/2} &= 1 \\ A^2(-a + \Delta a/2 + a + \Delta a/2) + 4A^2(a + \Delta a/2 - a + \Delta a/2) &= 1 \\ A^2\left(2\frac{\Delta a}{2}\right) + 4A^2(\Delta a) &= 1 \\ A^2 \cdot \Delta a + 4A^2 \cdot \Delta a &= 1 \\ \Delta a(5A^2) &= 1 \\ A^2 &= \frac{1}{5\Delta a} \\ A &= \frac{1}{\sqrt{5\Delta a}}. \end{aligned}$$

The spread in position can be calculated from,

$$(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle.$$

In order to calculate the mean value of x , i.e., $\langle x \rangle$, we use the wavefunction,

$$\begin{aligned} \langle x \rangle &= \int_{-a-\Delta a/2}^{-a+\Delta a/2} A dx + \int_{a-\Delta a/2}^{a+\Delta a/2} 2A dx \\ &= A(-a + \Delta a/2 + a + \Delta a/2) + 2A(a + \Delta a/2 - a + \Delta a/2) \\ &= A(\Delta a) + 2A(\Delta a) \\ &= 3A\Delta a. \end{aligned}$$

Substituting the value of A , we get,

$$\begin{aligned} \langle x \rangle &= 3 \frac{1}{\sqrt{5\Delta a}} \Delta a \\ \langle x \rangle &= 3\sqrt{\frac{\Delta a}{5}}. \end{aligned}$$

Equipped with these values, we calculate the spread in position,

$$\begin{aligned} x - \langle x \rangle &= \left(x - 3\sqrt{\frac{\Delta a}{5}} \right) \\ \Rightarrow (x - \langle x \rangle)^2 &= \left(x - 3\sqrt{\frac{\Delta a}{5}} \right)^2 \\ &= x^2 + \frac{9}{5}\Delta a - \frac{6}{\sqrt{5}}x\sqrt{\Delta a}. \end{aligned}$$

In order to calculate the mean value of the squared deviations, we proceed,

$$\begin{aligned} \langle (x - \langle x \rangle)^2 \rangle &= \int_{-a-\Delta a/2}^{-a+\Delta a/2} A^2 \left(x^2 + \frac{9}{5}\Delta a - \frac{6}{\sqrt{5}}x\sqrt{\Delta a} \right) dx + \\ &\quad \int_{a-\Delta a/2}^{a+\Delta a/2} (2A)^2 \left(x^2 + \frac{9}{5}\Delta a - \frac{6}{\sqrt{5}}x\sqrt{\Delta a} \right) dx \\ &= A^2 \left(\frac{x^3}{3} + \frac{9}{5}\Delta a x - \frac{6}{2\sqrt{5}}\sqrt{\Delta a} x^2 \right) \Big|_{-a-\Delta a/2}^{-a+\Delta a/2} \\ &\quad + 4A^2 \left(\frac{x^3}{3} + \frac{9}{5}\Delta a x - \frac{6}{2\sqrt{5}}\sqrt{\Delta a} x^2 \right) \Big|_{a-\Delta a/2}^{a+\Delta a/2} \\ &= A^2 \left[\left(\frac{1}{3}(-a + \Delta a/2)^3 + \frac{9}{5}\Delta a(-a + \Delta a/2) - \frac{6}{2\sqrt{5}}\sqrt{\Delta a}(-a + \Delta a/2)^2 \right) \right. \\ &\quad \left. - \left(\frac{1}{3}(-a - \Delta a/2)^3 + \frac{9}{5}\Delta a(-a - \Delta a/2) - \frac{6}{2\sqrt{5}}\sqrt{\Delta a}(-a - \Delta a/2)^2 \right) \right] \\ &\quad + 4A^2 \left[\left(\frac{1}{3}(a + \Delta a/2)^3 + \frac{9}{5}\Delta a(a + \Delta a/2) - \frac{6}{2\sqrt{5}}\sqrt{\Delta a}(a + \Delta a/2)^2 \right) \right. \\ &\quad \left. - \left(\frac{1}{3}(a - \Delta a/2)^3 + \frac{9}{5}\Delta a(a - \Delta a/2) - \frac{6}{2\sqrt{5}}\sqrt{\Delta a}(a - \Delta a/2)^2 \right) \right] \\ &= A^2 \left[\frac{5}{12}\Delta a^3 + 5a^2\Delta a + 9\Delta a^2 - \frac{18}{\sqrt{5}}a\Delta a^{3/2} \right] \\ &= \frac{1}{5\Delta a} \left[\frac{5}{12}\Delta a^3 + 5a^2\Delta a + 9\Delta a^2 - \frac{18}{\sqrt{5}}a\Delta a^{3/2} \right] \\ \langle (x - \langle x \rangle)^2 \rangle &= \frac{1}{12}\Delta a^2 + a^2 + \frac{9}{5}\Delta a - \frac{18}{5}a\Delta a. \end{aligned}$$

Which is the required result.

Answer 12.

Einstein's analysis of photoelectric effect shows that the maximum kinetic energy of photoelectrons is given by,

$$K_{max} = hf - w, \tag{1}$$

where w is the workfunction for given metal. Given are the maximum energies of the ejected photoelectrons,

$$K_1 = 8.57 \text{ eV} \quad \text{corresponding to ultra-violet light.}$$

$$K_2 = 6.67 \text{ eV} \quad \text{corresponding to blue-violet light.}$$

Using equation (1),

$$K_1 = \frac{hc}{\lambda_1} - w$$
$$K_2 = \frac{hc}{\lambda_2} - w.$$

Taking the difference of both these equations,

$$\begin{aligned} K_1 - K_2 &= \left(\frac{hc}{\lambda_1} - w\right) - \left(\frac{hc}{\lambda_2} - w\right) \\ &= \frac{hc}{\lambda_1} - \frac{hc}{\lambda_2} \\ &= hc\left(\frac{1}{\lambda_1} - \frac{1}{\lambda_2}\right) \\ &= hc\left(\frac{\lambda_1 - \lambda_2}{\lambda_1\lambda_2}\right) \\ \Rightarrow h &= \frac{(K_1 - K_2)\lambda_1\lambda_2}{c(\lambda_1 - \lambda_2)}. \end{aligned}$$

By plugging in the given values,

$$h = \frac{(8.57 - 6.67) \times 1.6 \times 10^{-19} \text{ J} \times (280 \times 10^{-9} \text{ m})(490 \times 10^{-9} \text{ m})}{3 \times 10^8 \text{ m/s} (490 - 280) \times 10^{-9} \text{ m}}$$
$$h \cong 6.63 \times 10^{-34} \text{ Js}.$$

Note that it is incorrect to equate the energy of the photoelectrons K with the incident energy of the photons, hc/λ .

Answer 13 :

Conservation of energy for the given collision requires that,

$$E_{initial} = E_{final}$$
$$hf + m_p c^2 = hf' + m_p c^2 + K,$$

where $m_p c^2$ is the rest mass energy of proton and K is the kinetic energy that is transferred

to the proton. The equation implies,

$$\begin{aligned}hf &= hf' + K \\ \frac{hc}{\lambda} &= \frac{hc}{\lambda'} + K \\ &= \frac{hc}{\lambda + \Delta\lambda} + K \\ K &= \frac{hc}{\lambda} - \frac{hc}{\lambda + \Delta\lambda} \\ \Rightarrow K &= \frac{hc\Delta\lambda}{\lambda(\lambda + \Delta\lambda)}.\end{aligned}\tag{2}$$

The change in wavelength is,

$$\Delta\lambda = \frac{h}{m_p c}(1 - \cos\theta).$$

Maximum energy goes to the proton when the photon's loss in energy is maximized. This happens when $\Delta\lambda$ is maximum. Therefore, the maximum change in wavelength occurs when $\theta = \pi$,

$$\begin{aligned}\Delta\lambda_{max} &= \frac{h}{m_p c}(1 - \cos\pi) \\ &= \frac{h}{m_p c}(1 - (-1)) \\ \Delta\lambda_{max} &= \frac{2h}{m_p c}\end{aligned}$$

Substituting this into equation (2), we get

$$\begin{aligned}K &= \frac{hc\left(\frac{2h}{m_p c}\right)}{\lambda\left(\lambda + \frac{2h}{m_p c}\right)} \\ &= \frac{hf\left(\frac{2h}{m_p c}\right)}{\left(\lambda + \frac{2h}{m_p c}\right)} \\ &= \frac{hf}{1 + \frac{m_p c \lambda}{2h}} \\ &= \frac{hf}{1 + \frac{m_p c^2}{2hf}}\end{aligned}$$

This is the expression for the maximum K.E transferred to photon.

Second method:

The kinetic energy that is transferred to the proton will be equal to the difference between the initial and final photon energies, i.e.,

$$K = hf - hf' \quad (3)$$

To find f' , we use the results of Compton effect.

$$\begin{aligned}\lambda' - \lambda &= \frac{h}{m_p c} (1 - \cos \theta) \\ \lambda' &= \lambda + \frac{h}{m_p c} (1 - \cos \theta) \\ \frac{c}{f'} &= \frac{c}{f} + \frac{h}{m_p c} (1 - \cos \theta) \\ \frac{1}{f'} &= \frac{1}{f} + \frac{h}{m_p c^2} (1 - \cos \theta) \\ \frac{1}{f'} &= \frac{m_p c^2 + hf(1 - \cos \theta)}{m_p c^2 \cdot f} \\ f' &= \frac{m_p c^2 \cdot f}{m_p c^2 + hf(1 - \cos \theta)} \\ f' &= \frac{f}{1 + \frac{hf(1 - \cos \theta)}{m_p c^2}}\end{aligned}$$

Substitute value of f' in equation (3), we get,

$$\begin{aligned}K &= hf - h \frac{f}{1 + \frac{hf(1 - \cos \theta)}{m_p c^2}} \\ &= hf \left(1 - \frac{1}{1 + \frac{hf(1 - \cos \theta)}{m_p c^2}} \right) \\ &= hf \left(\frac{1 + \frac{hf(1 - \cos \theta)}{m_p c^2} - 1}{1 + \frac{hf(1 - \cos \theta)}{m_p c^2}} \right) \\ &= hf \left(\frac{\frac{hf(1 - \cos \theta)}{m_p c^2}}{1 + \frac{hf(1 - \cos \theta)}{m_p c^2}} \right) \\ &= hf \frac{1}{\frac{m_p c^2}{hf(1 - \cos \theta)} + 1} \\ \Rightarrow K &= \frac{hf}{1 + \frac{m_p c^2}{hf(1 - \cos \theta)}}\end{aligned}$$

K is maximum when $\cos \theta = -1$, which is possible only at $\theta = \pi$, so,

$$K = \frac{hf}{1 + \frac{m_p c^2}{2hf}}$$

This will be expression of maximum kinetic energy that can be transferred to a proton, in terms of frequency. One can verify that this expression is identical to the one, calculated before.

Answer 14 :

a). Using the uncertainty principle,

$$\begin{aligned}\Delta E \cdot \Delta t &\geq \frac{\hbar}{2} \\ \Delta E \cdot \Delta t &\approx \frac{\hbar}{2}.\end{aligned}\tag{4}$$

To calculate the kinetic energy of an electron whose speed is 10 m/sec, with an uncertainty 0.1% , we use,

$$\begin{aligned}\Delta E &= \frac{0.1}{100} \times E \\ &= \frac{0.1}{100} \times \frac{1}{2}mv^2 \\ &= \frac{0.1}{100} \times \frac{1}{2} \times (9.11 \times 10^{-31} \times (10)^2) \\ \Delta E &= 4.55 \times 10^{-32} \text{J}\end{aligned}$$

Using equation (3),

$$\begin{aligned}\Delta t &\approx \frac{\hbar}{2\Delta E} \\ &\approx \frac{1.054 \times 10^{-34} \text{J sec}}{2 \times 4.55 \times 10^{-32} \text{J}} \\ &\approx 1 \times 10^{-3} \text{sec}.\end{aligned}$$

b). The distance covered by the electron during this time interval will be,

$$\begin{aligned}s &= v \Delta t \\ &= 10 \times 1.16 \times 10^{-3} \text{m} \\ s &= 0.01 \text{m}.\end{aligned}$$

Answer 15 :

a). The reduced mass of the revolving quark will be equal to,

$$\begin{aligned}\text{Reduced mass} &= \mu = \frac{m \cdot m}{m + m} = \frac{m^2}{2m} = \frac{m}{2} \\ \Rightarrow \mu &= \frac{m}{2}.\end{aligned}$$

b. Using the quantization of angular momentum, one can deduce,

$$\begin{aligned} L &= \mu v r = n \hbar \\ \Rightarrow r &= \frac{n \hbar}{\mu v} \end{aligned} \quad (5)$$

It is given that the centripetal centripetal force F is constant. i.e.,

$$\begin{aligned} F &= \frac{\mu v^2}{r} = \text{constant} = A \\ \Rightarrow v^2 &= \frac{r A}{\mu} \\ v &= \sqrt{\frac{r A}{\mu}} \end{aligned}$$

Substituting the value in equation (5), we get,

$$\begin{aligned} r &= \frac{n \hbar}{\mu \sqrt{\frac{r A}{\mu}}} \\ &= \frac{n \hbar}{\sqrt{\mu r A}} \\ \Rightarrow r^{3/2} &= \frac{n \hbar}{\sqrt{\mu A}} \\ r &= \frac{(n \hbar)^{2/3}}{(\mu A)^{1/3}} \\ r_n &= n^{2/3} \left(\frac{\hbar^2}{\mu A} \right)^{1/3}, \end{aligned}$$

which clearly shows that the radius is quantized, even though it is not proportional to n , rather to $n^{2/3}$. For smallest orbit, $n = 1$,

$$r_1 = \left(\frac{\hbar^2}{\mu A} \right)^{1/3}.$$

c). If the radius of the first orbit is r_1 , then the radius of the second orbit will be,

$$r_2 = 2^{2/3} r_1.$$

d). To calculate the quantized total energy, we take,

$$\begin{aligned} E &= K.E + P.E \\ &= \frac{1}{2} \mu v^2 + V(r). \end{aligned} \quad (6)$$

Now the potential energy is calculated from,

$$F = -\frac{dV(r)}{dr} = \text{constant} = A,$$

by integration

$$V(r) = -Ar.$$

Use value of potential energy in equation (6) and r_n from above expressions,

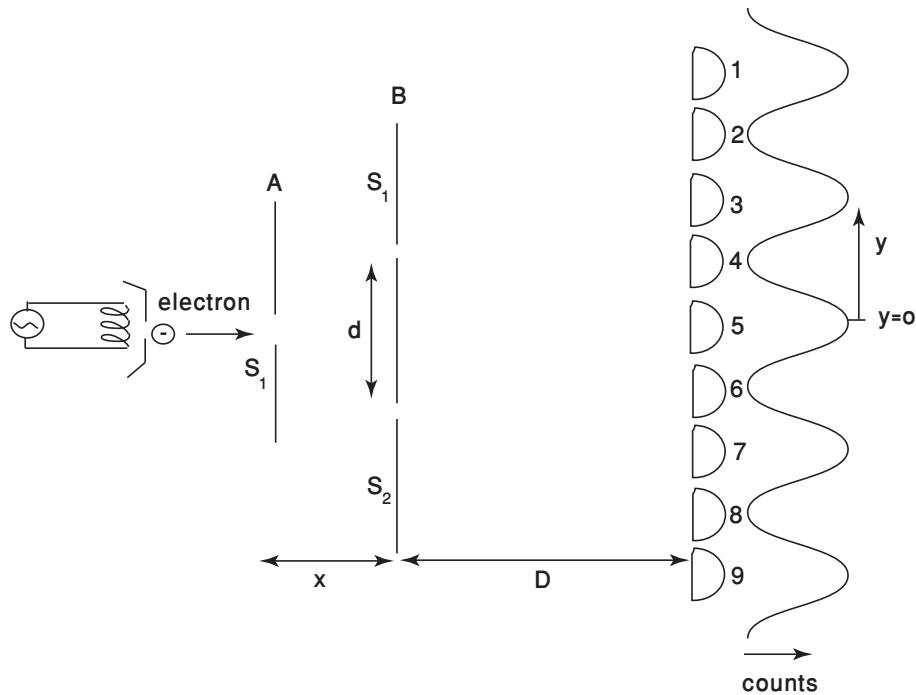
$$\begin{aligned} E &= \frac{1}{2}\mu v^2 - Ar_n \\ &= \frac{1}{2}\mu\left(\frac{r_n A}{\mu}\right) - Ar_n \\ &= \frac{1}{2}r_n A - Ar_n \\ &= -\frac{1}{2}r_n A \\ E_n &= -\frac{1}{2}n^{2/3}A\left(\frac{\hbar^2}{\mu A}\right)^{1/3}. \end{aligned}$$

where A is some constant equal to centripetal force. The dependence of E on the quantum number n is,

$$\Rightarrow E_n \propto n^{2/3},$$

showing that the total energy is also quantized and proportional to $n^{2/3}$.

Consider an experiment in which an electron source is placed in front of screens A and B . A has a narrow slit S_1 , B has two slits S_1 and S_2 . Detectors are placed at a distance D from B , and are numbered from 1 to N . The clicks registered by each detector are counted and at the end of the day-long experiment the counts are plotted.



The pattern of the counts is shown in the rightmost part of the diagram. The detectors are coincident with the maxima and the minima of the fringes. The source emits only one electron at a time and the time between consecutive electron emissions $\Delta t > (D + x)/c$, where c is the speed of light. Now answer the following questions.

1. Which of the following statements is true?
 - A. At one instant, all odd numbered detectors click together.
 - B. At one instant, all even numbered detectors click together.
 - C. More than one detector click at a time.
 - D. At one instant, only one of the odd-numbered detectors clicks.

E. None of the above are correct.

2. The fringes shown to the right of the detector array represent: (3 Marks)

A. The electric field of a single electron.

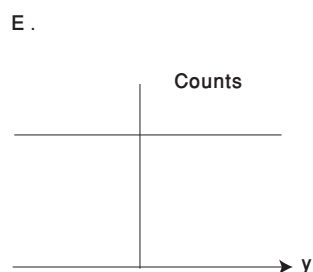
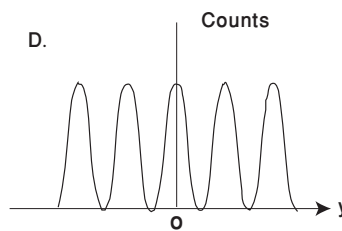
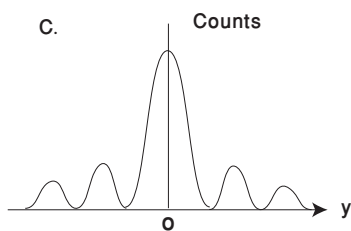
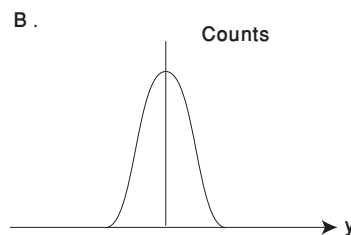
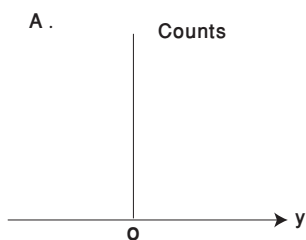
B. The momentum of a large number of electrons.

C. The wavefunction of a single electron $\psi(y)$.

D. The probability of the detectors clicking as a single electron traverses the apparatus.

E. The probability of the detectors clicking *after* many electrons have traveled through the apparatus.

3. If the screen B is completely removed, what form of the distribution of counts would you expect?



4. The visibility of the fringes is defined as:

$$\frac{C_{max} - C_{min}}{C_{max} + C_{min}}$$

where C_{max} is the maximum number of counts registered by any detector and C_{min} is the minimum number of counts. In this way, the visibility represents the contrast of the fringes. Now, if the experiment is allowed to run for 12 hours instead of 24 hours, what will happen to the visibility of the fringes?

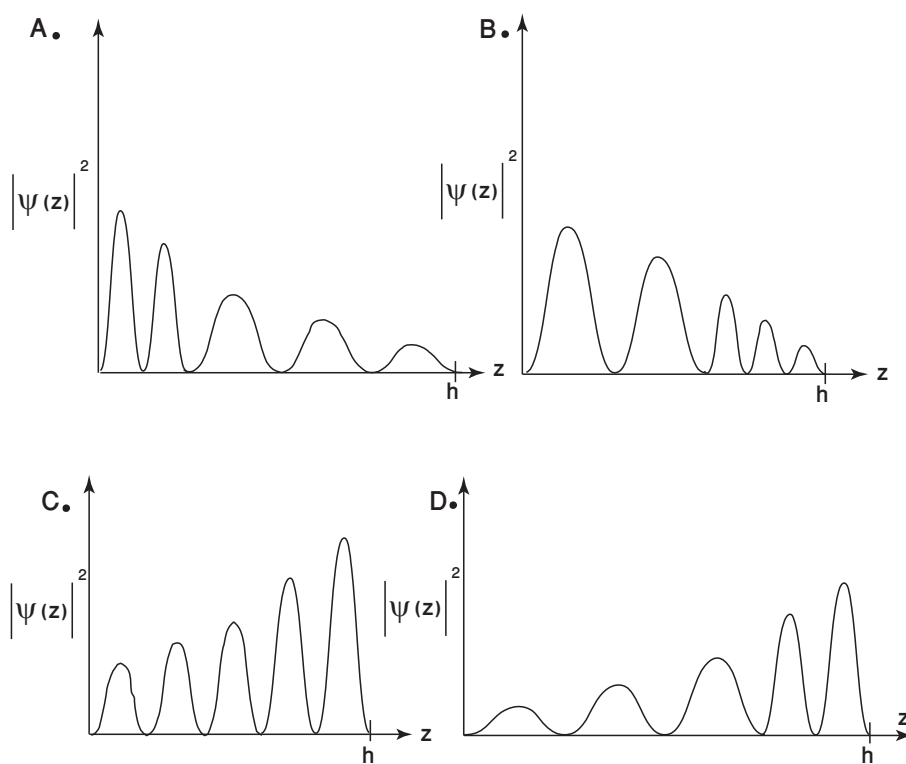
- A. It will have no effect as the fringes are formed by the interference of a single electron.
 - B. The visibility will double as we are now measuring for only half the time, and decreasing the time for which we disturb the system.
 - C. The visibility will halve.
 - D. We will not see any interference pattern at all.
 - E. None of the above.
5. The electrons are now replaced by neutrons moving with the same speed. How does the spacing between the maxima in the interference pattern change?
- A. The spacing increases.
 - B. The spacing decreases.
 - C. The spacing remains unchanged
 - D. The fringes will disappear altogether because the neutrons do not carry an electric charge.
 - E. None of the above.
6. An adventurous experimenter sets out to demonstrate interference for C_{60} molecules. His experiment is undoubtedly more difficult than electrons. He will have a better chance of observing interference fringes:
- A. By increasing the inter-slit distance d .
 - B. By decreasing both the distances d and D .

C. By increasing the ratio D/d .

D. By increasing the velocity of the C_{60} molecules.

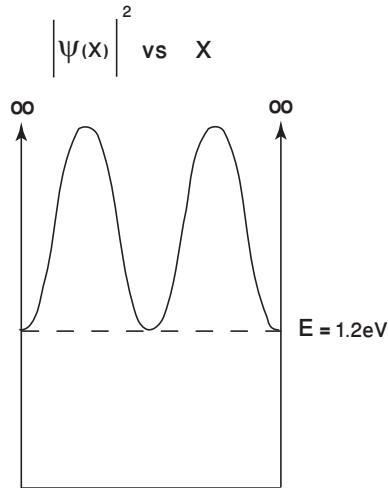
E. By allowing only one C_{60} molecule to pass through the apparatus.

7. In an experiment, a calcium ion Ca^{2+} is dropped from a height h . It falls under the action of gravity and rebounds from a flat surface (at $z = 0$) back up to the same height. There is no loss of energy anywhere. Which of these plots would be the best representation of the probability density $|\psi(z)|^2$ versus z , of a particular eigenstate of the system?



E. None of the above.

8. A particle is in an infinite potential well. It is in an eigenstate such that its probability density $|\psi(x)|^2$ versus x is shown here.



The energy of the state is 1.2 eV. What is the energy of the lowest possible allowed energy state in this well? (3 Marks)

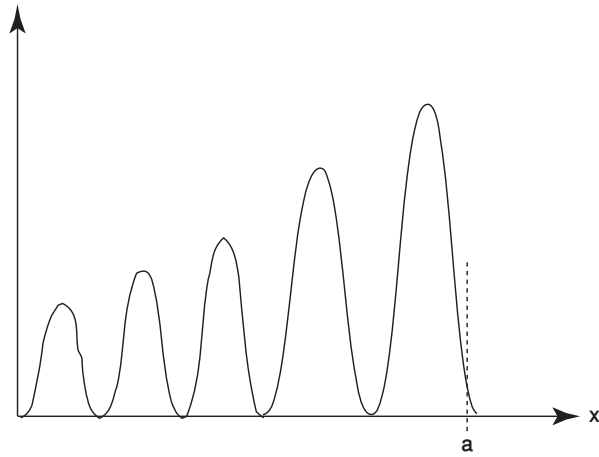
- A. 0.0 eV
- B. 0.3 eV
- C. 0.6 eV
- D. 1.2 eV
- E. We cannot be certain of the lowest energy state.

9. The position wavefunction, $\psi(x)$ of a particle at some instant is given by,

$$\psi(x) = \frac{1}{L^2 + (x - x_o)^2/\alpha^2},$$

where L, x_o, α are constants. Which of the following expression below is a good approximate to the spread in the momentum, Δp ?

- A. $\Delta p \sim \hbar/(\alpha L)$
- B. $\Delta p \sim \hbar/\alpha$
- C. $\Delta p \sim \hbar/(\alpha^2 x_o)$
- D. $\Delta p \sim \hbar/(\alpha^2 L^2)$
- E. $\Delta p \sim \hbar/(\alpha x_o)$



10. The probability density of a particle of energy E is shown in the diagram.

The particle is trapped inside a triangular potential well. Which of the following is the most likely form of the potential well? **See the next page for the potentials.**

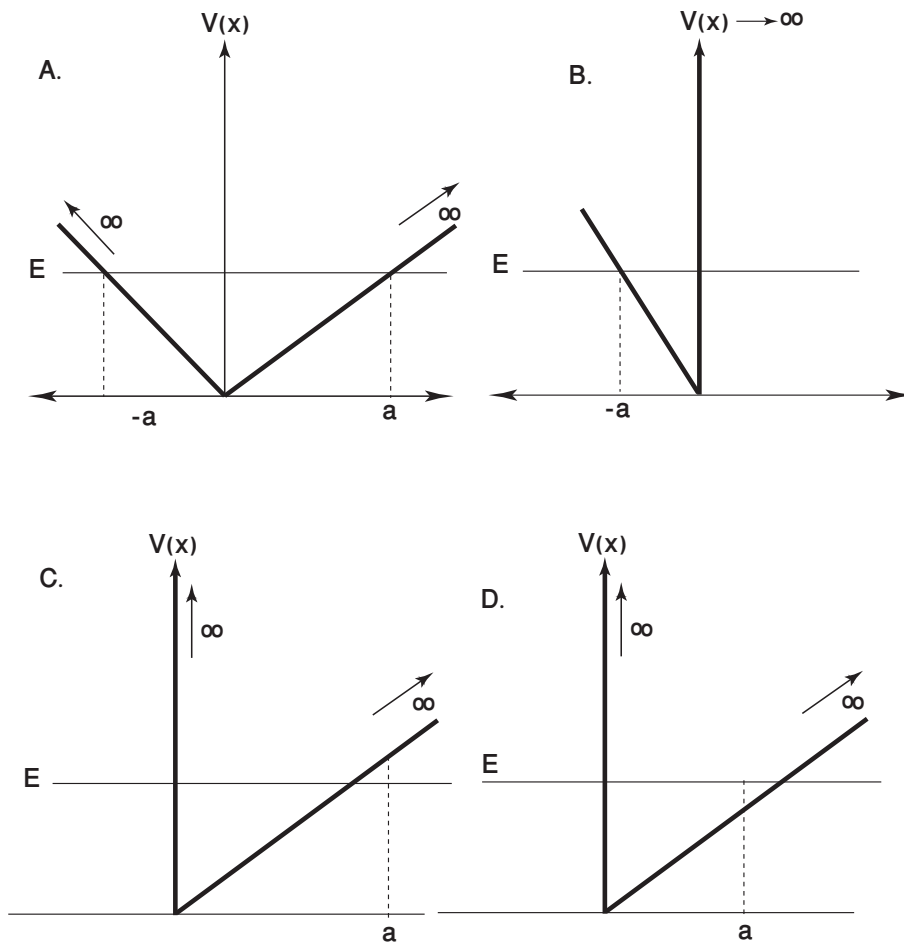


FIG. 1: Figure for Q. 10.

Assignment 6: Potential Steps, Barriers and Wells

1. Sketch a possible solution to the Schrodinger equation for each of the potential energy functions shown in the diagram. In each case, show several cycles of the wavefunction.

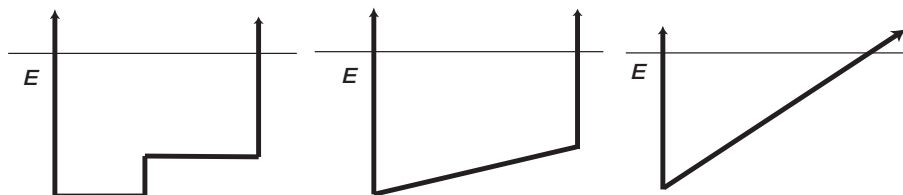


FIG. 1: Figure for Question 1.

2. An electron is trapped inside a one-dimensional well of width 0.132 nm. The electron is in the $n = 10$ state. (a) What is the energy of the electron? (b) What is the uncertainty in its momentum? (c) What is the uncertainty in its position? (d) How do these results change as $n \rightarrow \infty$? Is this consistent with classical behaviour?
3. Consider a beam of electrons passing through a cell containing atoms of the rare gas krypton. The krypton atoms present a potential well of depth V_0 as shown in the figure.

(a) Show that the transmissivity T of the electrons is given by,

$$\frac{1}{T} = 1 + \frac{1}{4} \frac{V_0^2}{E(E + V_0)} \sin^2(k_2 a), \quad (1)$$

where k_2 is the wavenumber inside the well.

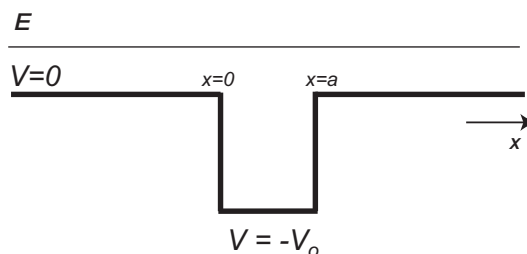


FIG. 2: Figure for Question 3.

Assignment 6: Potential Steps, Barriers and Wells

- (b) The reflection of the electrons exhibits the lowest-energy minimum at 0.9 eV. Assuming that the diameter of the krypton atom is approximately one Bohr's radius, calculate the depth of the well.
4. In the phenomenon of cold emission, electrons are drawn from a metal when placed inside an electric field ϵ . The electrons are present in the conduction band within the metal and range up to energies E_f called the Fermi energy. The potential barrier, depicted in the accompanying figure, presents a triangular slope. The metal-vacuum interface is at $x = 0$.
- (a) Why is the potential energy sloping downwards in the region of the vacuum, $x > 0$? What is the field inside the metal, $x < 0$?
- (b) Suppose the tunneling probability is given by $T \approx \exp\left(-2\sqrt{\frac{2m(V(x)-E)}{\hbar}}\right)$. What is the probability that a Fermi electron can tunnel through the barrier?
- (c) A gold tip (work function $w = 4.5$ eV) is used in a cold field emission electron microscope. Calculate the electric field ϵ required to allow a tunneling probability of 10^{-4} .

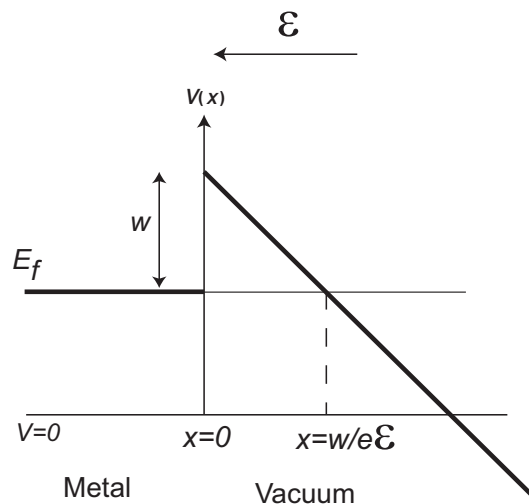
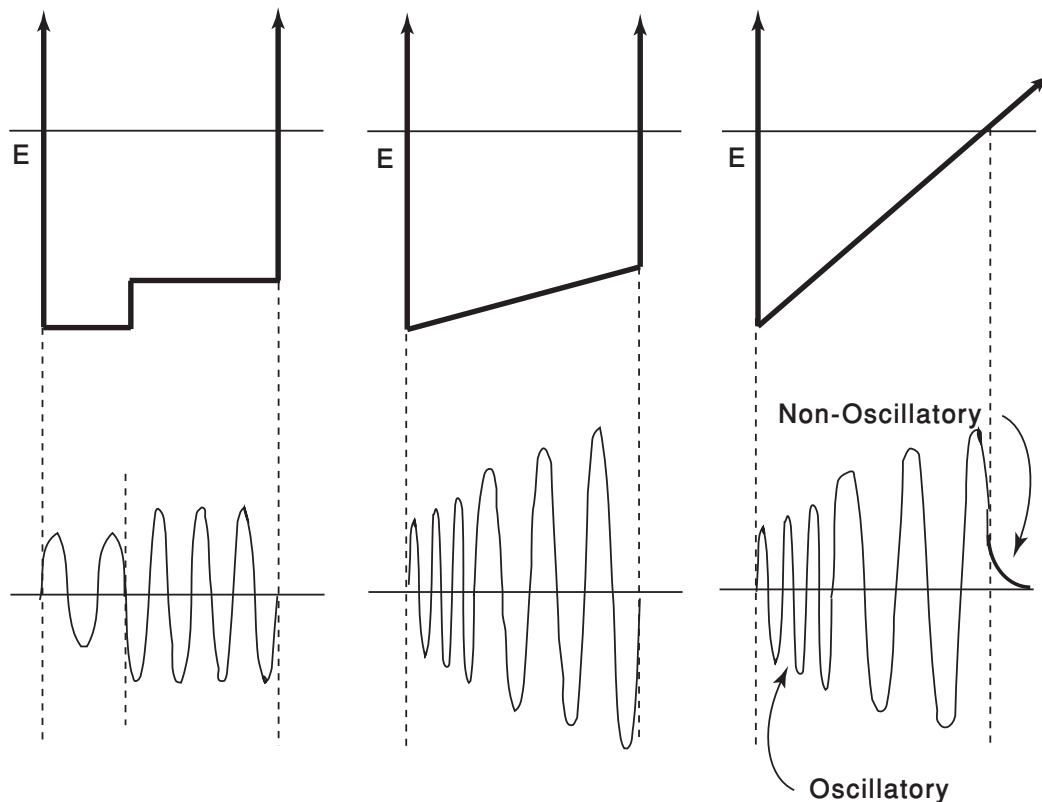


FIG. 3: Figure for Question 4.

Potential Steps, Barriers and Wells

Answer 1.



Answer 2.

(a)

The total quantized energy inside the well (which equals its kinetic energy) is,

$$E = \frac{\pi^2 \hbar^2 n^2}{2ma^2} \quad (1)$$

$$E = 2.1 \text{ MeV}.$$

(b)

The momentum of the electron can have only two values inside the well. i.e.,

$$p = \pm \sqrt{2mE},$$

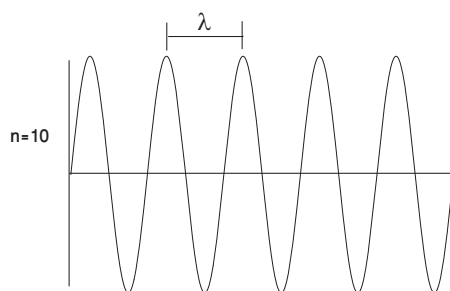
showing that we cannot tell which direction the electron is moving. Therefore, the uncertainty in momentum will be of the order of p and we can say, $\Delta p \approx p$.

(c)

To find out the uncertainty in position,

$$\begin{aligned}\Delta p \Delta x &\approx \hbar \\ \Delta x &\approx \frac{\hbar}{\Delta p} \\ \Delta x &\approx \frac{\hbar}{p} \\ &\approx \frac{h}{2\pi p} \\ \Delta x &\approx \frac{\lambda}{2\pi}\end{aligned}$$

i.e., the uncertainty in the position is of electron is of the order its wavelength. Since the



momentum inside the well is given by,

$$p = \pm\sqrt{2mE},$$

substituting the value of E from equation (1), results in,

$$\begin{aligned}\Delta p = p &= \sqrt{2m} \frac{\pi \hbar n}{\sqrt{2m} a} \\ &= \frac{\pi \hbar n}{a}.\end{aligned}$$

The uncertainty in position is,

$$\begin{aligned}\Delta x &\approx \frac{\hbar a}{\pi \hbar n} \\ \Delta x &\approx \frac{a}{\pi n} \\ \Delta x &\approx \frac{0.132 \text{ nm}}{3.14 \times 10} \\ \Delta x &\approx 4.2 \times 10^{-12} \text{ m},\end{aligned}\tag{2}$$

which is of the same order as the wavelength! (**Check this.**)

(d) From Equation 2, we see that as $n \rightarrow \infty$, $\Delta x \rightarrow 0$: we can precisely locate the particle, consistent with classical behaviour. High n states correspond to the classical scenario, large values of n imply large energies as compared to the ground state energy. This is immediately evident from Equation 1.

Answer 3.

(a)

The general solution of the Schrodinger wave equation in the three regions is given by,

$$\psi(x) = \begin{cases} \psi_1(x) = A e^{(ik_1x)} + B e^{(-ik_1x)} & x \leq 0 \\ \psi_2(x) = C e^{(ik_2x)} + D e^{(-ik_2x)} & 0 < x < a \\ \psi_3(x) = E e^{(ik_2x)} & x \geq a \end{cases}$$

Where $k_1 = \frac{\sqrt{2mE}}{\hbar}$ and $k_2 = \frac{\sqrt{2m(E - (-V_o))}}{\hbar}$. In order to findout the transmissivity T of the electron, we use the appropriate boundary conditions.

At $x = 0$,

$$\begin{aligned} \psi_1(x = 0) &= \psi_2(x = 0) \\ \frac{d\psi_1(x = 0)}{dx} &= \frac{d\psi_2(x = 0)}{dx} \end{aligned}$$

At $x = a$, we have,

$$\begin{aligned} \psi_2(x = a) &= \psi_3(x = a) \\ \frac{d\psi_2(x = a)}{dx} &= \frac{d\psi_3(x = a)}{dx} \end{aligned}$$

Using the definition of wavefunction, we get the following equations,

$$A + B = C + D \tag{3}$$

$$ik_1(A - B) = ik_2(C - D) \tag{4}$$

$$C e^{ik_2a} + D e^{-ik_2a} = E e^{ik_1a} \tag{5}$$

$$ik_2(C e^{ik_2a} - D e^{-ik_2a}) = ik_1(E e^{ik_1a}). \tag{6}$$

Equation (4) can also be written as,

$$A - B = \frac{k_2}{k_1} (C - D). \tag{7}$$

Adding equation (3) and (7), we get,

$$2A = (C + D) + \frac{k_2}{k_1}(C - D). \quad (8)$$

Similarly, equation (6) can be written as,

$$Ce^{ik_2a} - De^{-ik_2a} = \frac{k_1}{k_2}Ee^{ik_1a}. \quad (9)$$

Adding equation (4) and (9), we get

$$\begin{aligned} 2Ce^{ik_2a} &= Ee^{ik_1a} \left\{1 + \frac{k_1}{k_2}\right\} \\ C &= \frac{E}{2} \left\{1 + \frac{k_1}{k_2}\right\} e^{i(k_1-k_2)a}, \end{aligned}$$

subtracting equation (4) and (9) yields,

$$\begin{aligned} 2De^{-ik_2a} &= Ee^{ik_1a} \left\{1 - \frac{k_1}{k_2}\right\} \\ D &= \frac{E}{2} \left\{1 - \frac{k_1}{k_2}\right\} e^{i(k_1-k_2)a}. \end{aligned}$$

substitute values of C and D in equation (8), we get,

$$\begin{aligned} 2A &= \left(\frac{E}{2} \left\{1 + \frac{k_1}{k_2}\right\} e^{i(k_1-k_2)a} + \frac{E}{2} \left\{1 - \frac{k_1}{k_2}\right\} e^{i(k_1-k_2)a} \right) \\ &+ \frac{k_2}{k_1} \left(\frac{E}{2} \left\{1 + \frac{k_1}{k_2}\right\} e^{i(k_1-k_2)a} - \frac{E}{2} \left\{1 - \frac{k_1}{k_2}\right\} e^{i(k_1-k_2)a} \right) \\ &= \frac{E}{2} \left(1 + \frac{k_1}{k_2}\right) e^{i(k_1-k_2)a} \left(1 + \frac{k_2}{k_1}\right) + \frac{E}{2} \left(1 - \frac{k_1}{k_2}\right) e^{i(k_1-k_2)a} \left(1 - \frac{k_2}{k_1}\right) \\ &= \frac{E}{2} e^{i(k_1-k_2)a} \left(1 + \frac{k_1}{k_2}\right) \left(1 + \frac{k_2}{k_1}\right) + \frac{E}{2} e^{i(k_1-k_2)a} \left(1 - \frac{k_1}{k_2}\right) \left(1 - \frac{k_2}{k_1}\right) \\ &= \frac{E}{2} e^{i(k_1-k_2)a} \left(\frac{k_1+k_2}{k_2}\right) \left(\frac{k_1+k_2}{k_1}\right) + \frac{E}{2} e^{i(k_1-k_2)a} \left(\frac{k_2-k_1}{k_2}\right) \left(\frac{k_1-k_2}{k_1}\right) \\ &= \frac{E}{2k_1k_2} (k_1+k_2)^2 e^{i(k_1-k_2)a} - \frac{E}{2k_1k_2} (k_1-k_2)^2 e^{i(k_1-k_2)a} \\ 2A &= \frac{E}{2k_1k_2} \left((k_1+k_2)^2 e^{i(k_1-k_2)a} - (k_1-k_2)^2 e^{i(k_1-k_2)a} \right) \\ \frac{E}{A} &= \frac{4k_1k_2 e^{-ik_1a}}{(k_1+k_2)^2 e^{-ik_2a} - (k_1-k_2)^2 e^{-ik_2a}}. \end{aligned}$$

This denominator can further be simplified as,

$$\begin{aligned}
 &= (k_1 + k_2)^2 e^{-ik_2a} - (k_1 - k_2)^2 e^{-ik_2a} \\
 &= (k_1^2 + k_2^2 + 2k_1k_2) e^{-ik_2a} - (k_1^2 + k_2^2 - 2k_1k_2) e^{ik_2a} \\
 &= (k_1^2 + k_2^2) e^{-ik_2a} - (k_1^2 + k_2^2) e^{ik_2a} + 2k_1k_2 e^{-ik_2a} + 2k_1k_2 e^{ik_2a} \\
 &= 2 \times 2k_1k_2 \left(\frac{e^{ik_2a} + e^{-ik_2a}}{2} \right) - 2i(k_1^2 + k_2^2) \left(\frac{e^{ik_2a} - e^{-ik_2a}}{2i} \right) \\
 &= 4k_1k_2 \cos(k_2a) - 2i(k_1^2 + k_2^2) \sin(k_2a).
 \end{aligned}$$

Therefore,

$$\begin{aligned}
 \frac{E}{A} &= \frac{4k_1k_2 e^{-ik_1a}}{4k_1k_2 \cos(k_2a) - 2i(k_1^2 + k_2^2) \sin(k_2a)} . \\
 \frac{E^*}{A^*} &= \frac{4k_1k_2 e^{ik_1a}}{4k_1k_2 \cos(k_2a) + 2i(k_1^2 + k_2^2) \sin(k_2a)} .
 \end{aligned}$$

Transmissivity is given by,

$$\begin{aligned}
 T &= \frac{E^*E}{A^*A} \\
 &= \frac{4k_1k_2 e^{-ik_1a}}{4k_1k_2 \cos(k_2a) - 2i(k_1^2 + k_2^2) \sin(k_2a)} \times \frac{4k_1k_2 e^{ik_1a}}{4k_1k_2 \cos(k_2a) + 2i(k_1^2 + k_2^2) \sin(k_2a)} \\
 T &= \frac{16k_1^2k_2^2}{16k_1^2k_2^2 \cos^2(k_2a) + 4(k_1^2 + k_2^2)^2 \sin^2(k_2a)} .
 \end{aligned}$$

The denominator can further be simplified as,

$$\begin{aligned}
 &= 16k_1^2k_2^2 \cos^2(k_2a) + 4(k_1^2 + k_2^2)^2 \sin^2(k_2a) \\
 &= 16k_1^2k_2^2 \cos^2(k_2a) + 4(k_1^4 + k_2^4 + 2k_1^2k_2^2) \sin^2(k_2a) \\
 &= 16k_1^2k_2^2 (\cos^2(k_2a) + \sin^2(k_2a)) + 4(k_1^4 + k_2^4) \sin^2(k_2a) \\
 &= 16k_1^2k_2^2 + 4(k_1^4 + k_2^4) \sin^2(k_2a) .
 \end{aligned}$$

Transmission coefficient becomes,

$$\begin{aligned}
 T &= \frac{16k_1^2k_2^2}{16k_1^2k_2^2 + 4(k_1^4 + k_2^4) \sin^2(k_2a)} \\
 &= \frac{1}{1 + \frac{1}{4} \left(\frac{k_1^4 + k_2^4}{k_1^2k_2^2} \right) \sin^2(k_2a)} \\
 T &= \frac{1}{1 + \frac{1}{4} \left(\frac{k_1^2 - k_2^2}{k_1^2k_2^2} \right)^2 \sin^2(k_2a)} .
 \end{aligned}$$

Since, $k_1 = \frac{\sqrt{2mE}}{\hbar}$ and $k_2 = \frac{\sqrt{2m(E+V_0)}}{\hbar}$, substituting values into the denominator,

$$\begin{aligned} \frac{k_1^2 - k_2^2}{k_1^2 k_2^2} &= \frac{\frac{2mE}{\hbar^2} - \frac{2m(E+V_0)}{\hbar^2}}{\frac{\sqrt{2mE}}{\hbar} \frac{\sqrt{2m(E+V_0)}}{\hbar}} \\ &= \frac{\frac{2mE - 2m(E+V_0)}{\hbar^2}}{\frac{\sqrt{2m}\sqrt{2m}}{\hbar^2} \sqrt{E(E+V_0)}} \\ &= \frac{-2mV_0}{\hbar^2} \times \frac{\hbar^2}{2m\sqrt{E(E+V_0)}} \\ &= \frac{-V_0}{\sqrt{E(E+V_0)}}. \end{aligned}$$

Therefore, transmissivity is,

$$\begin{aligned} T &= \frac{1}{1 + \frac{1}{4} \left(\frac{-V_0}{\sqrt{E(E+V_0)}} \right)^2 \sin^2(k_2 a)} \\ &= \frac{1}{1 + \frac{1}{4} \left(\frac{V_0^2}{E(E+V_0)} \right) \sin^2(k_2 a)} \\ \frac{1}{T} &= 1 + \frac{1}{4} \left(\frac{V_0^2}{E(E+V_0)} \right) \sin^2(k_2 a), \end{aligned}$$

where k_2 is the wavenumber inside the well. This is our desired result.

(b)

Since the reflection of the electrons exhibits the lowest-energy minimum at 0.9 eV, we assume that at this energy, $R = 0$ and $T = 1$. Therefore,

$$\begin{aligned} 1 &= 1 + \frac{1}{4} \left(\frac{V_0^2}{E(E+V_0)} \right) \sin^2(k_2 a) \\ 0 &= \frac{1}{4} \left(\frac{V_0^2}{E(E+V_0)} \right) \sin^2(k_2 a) \end{aligned}$$

Since $V_0^2 \neq 0$, $\sin^2(k_2 a) = 0$, requiring,

$$\begin{aligned} k_2 a &= n\pi \\ k_2 &= \frac{n\pi}{a} \end{aligned}$$

Assuming that the first maxima occurs at $n = 1$,

$$\begin{aligned} k_2 &= \frac{\pi}{a} \\ \frac{\sqrt{2m(E + V_0)}}{\hbar} &= \frac{\pi}{a} \\ 2m(E + V_0) &= \frac{\pi^2 \hbar^2}{a^2} \\ V_0 &= \frac{\pi^2 \hbar^2}{2ma^2} - E \end{aligned}$$

Assuming a to be the Bohr's radius, $a \simeq 0.5 \text{ \AA}$, substitute values,

$$\begin{aligned} V_0 &= \frac{(3.14)^2 (1.054 \times 10^{-34})^2}{2(9.11 \times 10^{-31})(0.5 \times 10^{-10})^2} - 0.9 \times 1.6 \times 10^{-19} \\ V_0 &= 150 \text{ eV}. \end{aligned}$$

This will be the depth of the well, which will ensure perfect tunneling (transmission) of the electrons through the Kr atoms. It is as good as the complete absence of Kr atoms!

Answer 4.

(a)

The electric field is in the direction of decreasing x (to the left), so,

$$\begin{aligned} e\varepsilon &= \frac{-dV}{dx} \\ V &= -e\varepsilon x, \end{aligned}$$

i.e., the potential energy increases as x decreases. That's why in the region of vacuum, the potential energy is sloping downward.

Further, inside the metal, the charges are at rest and the potential is uniform over there, therefore, the electric field inside the metal is equal to zero.

(b)

To calculate the probability that a (Fermi) electron can tunnel through the barrier, we divide the region from $x = 0$ to $x = w/e\varepsilon$ into small parts and integrate over the whole region.

Given is

$$T \approx \exp\left(\frac{-2}{\hbar} \sqrt{2m(V(x) - E_f)} a\right).$$

The potential is given by, (use the equation of line, slope is $m = \frac{-w}{w/e\varepsilon} = -e\varepsilon$) and intercept

$$c = w + E_f,$$

$$y = mx + c$$

$$V(x) = -e\varepsilon x + w + E_f$$

$$V(x) - E_f = w - e\varepsilon x.$$

Transmission coefficient becomes,

$$T \approx \exp\left(\frac{-2}{\hbar} \sqrt{2m(w - e\varepsilon x)} a\right).$$

The tunneling probability will be equal to the product of transmission coefficient in each part, resulting in integration within the powers of exponential,

$$P \approx \exp\left(\frac{-2}{\hbar} \int_{x=0}^{w/e\varepsilon} \sqrt{2m(w - e\varepsilon x)} a dx\right).$$

Let,

$$u = w - e\varepsilon x$$

$$du = -e\varepsilon dx$$

$$dx = \frac{-1}{e\varepsilon} du,$$

$$\text{when } x = 0, \quad u = w, \quad \text{and}$$

$$\text{when } x = w/e\varepsilon, \quad u = 0.$$

Hence, the integration reduces to,

$$\begin{aligned} P &\approx \exp\left(\frac{+2}{e\varepsilon\hbar} \int_{u=w}^0 \sqrt{2mu} a du\right) \\ &\approx \exp\left(\frac{+2a\sqrt{2m}}{e\varepsilon\hbar} \int_{u=w}^0 \sqrt{u} du\right) \\ &\approx \exp\left(\frac{+2a\sqrt{2m}}{e\varepsilon\hbar} \frac{2}{3} u^{3/2} \Big|_w^0\right) \\ &\approx \exp\left(\frac{+4a\sqrt{2m}}{3e\varepsilon\hbar} (0 - w^{3/2})\right) \\ P &\approx \exp\left(\frac{-4a\sqrt{2m}}{3e\varepsilon\hbar} w^{3/2}\right). \end{aligned}$$

Hence the Fermi electron can tunnel through the barrier with this probability.

(d)

The Work function w of the gold tip is given by,

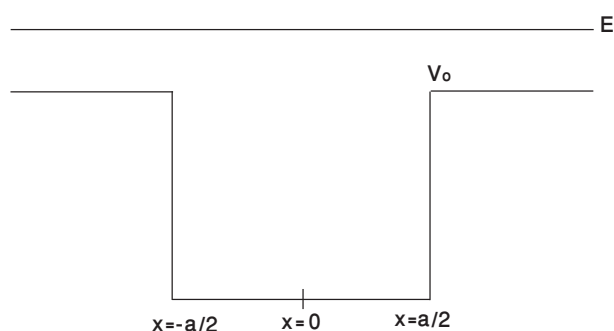
$$\begin{aligned}w &= 4.5 \text{ eV} \\ &= 4.5 \times 1.6 \times 10^{-19} \\ w &= 7.2 \times 10^{-19} \text{ J}.\end{aligned}$$

The electric field ϵ required to achieve $P \approx 10^{-4}$ is calculated as,

$$\begin{aligned}P &\approx \exp\left(\frac{-4 a \sqrt{2m}}{3e \epsilon \hbar} w^{3/2}\right) \\ \ln(P) &\approx \left(\frac{-4 a \sqrt{2m}}{3e \epsilon \hbar} w^{3/2}\right) \\ \epsilon &\approx \left(\frac{-4 a \sqrt{2m}}{3e \ln(P) \hbar} w^{3/2}\right) \\ &\approx \left(\frac{(-4 \times 0.53 \times 10^{-10}) \sqrt{2 \times 9.11 \times 10^{-31}}}{3(1.6 \times 10^{-19})(-4) \ln(10)(1.054 \times 10^{-34})} (7.2 \times 10^{-19})^{3/2}\right) \\ \epsilon &\approx 0.38 \text{ V/m}.\end{aligned}$$

Assignment 7: The finite wells and tunneling effect

1. A proton and a deuteron (a particle with the same charge as a proton, but twice the mass) attempt to penetrate a rectangular potential barrier of height 10 MeV and thickness 10^{-14} m. Both particles have total energies of 3 MeV. (a) Use qualitative arguments to predict which particle has the highest probability of succeeding. (b) Evaluate quantitatively the probability of success for both the particles.
2. Given is the following figure.



Make a quantitative calculation of the transmission coefficient for an unbound particle moving over a finite square well potential. (b) Find a condition on the total energy of the particle which makes the transmission coefficient equal to one. (c) Give an example of an optical analogue to this system.

3. Given is the normalized eigenfunction of infinite square well potential,

$$\psi_n(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right)$$

Calculate the following expectation values and comment on each result, (a) \bar{x} (b) \bar{p} (c) $\overline{x^2}$ (d) $\overline{p^2}$. (e) Use these results to evaluate the product of the uncertainty in position times the uncertainty in momentum, for a particle in the $n=3$ state of an infinite square well potential.

4. Two possible eigenfunctions for a particle moving freely in a region of length a , but strictly confined to that region, are shown in the figure below. When the particle is in the state corresponding to the eigenfunction ψ_I , its total energy is 4 eV. (a) What is its total energy in the state corresponding to ψ_{II} ? (b) What is the lowest possible total energy for the particle in this system?

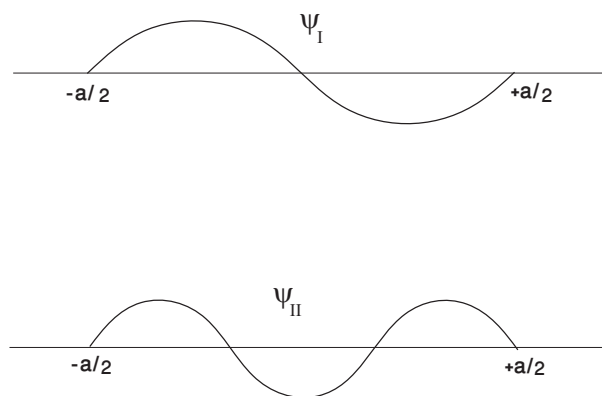


Fig. Two eigenfunctions considered in problem 4

5. A fusion reaction important in solar energy production involves capture of a proton by a carbon nucleus, which has six times the charge of a proton and a radius of $r' \simeq 2 \times 10^{-15}$ m. (a) Estimate the Coulomb potential V experienced by the proton if it is at the nuclear surface. (b) The proton is incident upon the nucleus because of its thermal motion. Its total energy cannot realistically be assumed to be higher than $10kT$, where k is Boltzmann's constant and where T is the internal temperature of the sun of about 10^7 °xK. Estimate this total energy, and compare it with the height of the Coulomb barrier. (c) Calculate the probability that the proton can penetrate a rectangular barrier potential of height V extending from r' to $2r'$, the point at which the Coulomb barrier potential drops to $V/2$. (d) Is the penetration through the actual Coulomb barrier potential greater or less than through the rectangular barrier potential of part (c).

Finite wells and tunneling effectAnswer 1.

(a)

The opacity of the barrier (the degree to which the particles are blocked) is directly proportional to mass of the particle. Hence, the lower mass particle (proton) has the high probability of getting through.

We can also support our argument with the help of expression for the transmission coefficient, which is case of rectangular potential barrier is given by,

$$T \simeq 16 \frac{E}{V_o} \left(1 - \frac{E}{V_o}\right) e^{-2k_2 a}, \quad \text{where,}$$

$$k_2 = \sqrt{\frac{2mV_o a^2 \left(1 - \frac{E}{V_o}\right)}{\hbar^2}}.$$

For massive particles, k_2 will be greater, as a result, the transmissivity will be lesser.

b). In order to find out the transmissivity or the probability of success for the protons, we use the expression of transmissivity of rectangular potential barrier,

$$T = \frac{1}{1 + \sinh^2(k_2 a) \left(\frac{k_1^2 + k_2^2}{2k_1 k_2}\right)}, \quad \text{where,}$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar}$$

$$k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \cot$$

In case of proton,

$$k_1 = \frac{\sqrt{2mE}}{\hbar} = \frac{\sqrt{2 \times 1.67 \times 10^{-27} \times 3 \times 10^6 \times 1.6 \times 10^{-19}}}{1.054 \times 10^{-34}}$$

$$= 3.7 \times 10^{14}.$$

$$k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar} = \frac{\sqrt{2 \times 1.67 \times 10^{-27} \times (10 - 3) \times 10^6 \times 1.6 \times 10^{-19}}}{1.054 \times 10^{-34}}$$

$$= 5.8 \times 10^{14}.$$

Hence, the transmission coefficient is,

$$\begin{aligned} T &= \frac{1}{1 + \sinh^2(5.8 \times 10^{14} \times 10^{-14}) \left(\frac{(3.7 \times 10^{14})^2 + (5.8 \times 10^{14})^2}{2 \times (3.7 \times 10^{14})(5.8 \times 10^{14})} \right)} \\ &= 3 \times 10^{-5}. \end{aligned}$$

Similarly, for deuteron, $m_d = 2m_p$, we get

$$\begin{aligned} k_1 &= \sqrt{2} \times 3.71 \times 10^{14} \\ &= 5.2 \times 10^{14} \\ k_2 &= \sqrt{2} \times 5.80 \times 10^{14} \\ &= 8.2 \times 10^{14}. \end{aligned}$$

The transmission coefficient for deuteron is,

$$\begin{aligned} T &= \frac{1}{1 + \sinh^2(8.2 \times 10^{14} \times 10^{-14}) \left(\frac{(5.2 \times 10^{14})^2 + (8.2 \times 10^{14})^2}{2 \times (5.2 \times 10^{14})(8.2 \times 10^{14})} \right)} \\ &= 2.5 \times 10^{-7}, \end{aligned}$$

which shows that the results are precisely in accordance with the previous one's.

Answer 2.

Given is the wave function,

$$\psi_3 = A \cos\left(\frac{3\pi x}{a}\right)$$

To find out the normalization constant A , we use the normalization condition,

$$\begin{aligned}
 \int \psi_3^*(x) \psi_3(x) dx &= 1 \\
 \int_{-a/2}^{a/2} A^2 \cos^2\left(\frac{3\pi x}{a}\right) dx &= 1 \\
 A^2 \int_{-a/2}^{a/2} \cos^2\left(\frac{3\pi x}{a}\right) dx &= 1 \\
 A^2 \int_{-a/2}^{a/2} \left(\frac{1 + \cos(2 \cdot 3\pi x/a)}{2}\right) dx &= 1 \\
 A^2 \int_{-a/2}^{a/2} \left[\frac{1}{2} + \frac{\cos(6\pi x/a)}{2}\right] dx &= 1 \\
 A^2 \left[\frac{1}{2} x \Big|_{-a/2}^{a/2} + \frac{1}{2} \cdot \frac{\sin(6\pi x/a)}{6\pi/a} \Big|_{-a/2}^{a/2} \right] &= 1 \\
 A^2 \left[\frac{1}{2} \left(\frac{a}{2} + \frac{a}{2}\right) + \frac{1}{2} \cdot \frac{a}{6\pi} \left(\sin\left(\frac{6\pi a}{2a}\right) - \sin\left(\frac{-6\pi a}{2a}\right)\right) \right] &= 1 \\
 A^2 \left[\frac{a}{2} + \frac{a}{12\pi} (\sin(3\pi) - \sin(-3\pi)) \right] &= 1 \\
 A^2 \left[\frac{a}{2} \right] &= 1 \\
 A^2 &= \frac{2}{a} \\
 A &= \sqrt{\frac{2}{a}},
 \end{aligned}$$

therefore, the normalized wavefunction is,

$$\psi_3(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{3\pi x}{a}\right).$$

a). The expectation value of the position is,

$$\begin{aligned}
 \langle x \rangle = \bar{x} &= \int_{-a/2}^{a/2} \psi_3^*(x) x \psi_3(x) dx \\
 &= \frac{2}{a} \int_{-a/2}^{a/2} x \cos^2\left(\frac{3\pi x}{a}\right) dx \\
 &= \frac{2}{a} \int_{-a/2}^{a/2} x \left(\frac{1 + \cos\left(\frac{2 \cdot 3\pi x}{a}\right)}{2}\right) dx \\
 &= \frac{2}{a} \int_{-a/2}^{a/2} \left(\frac{x}{2} + \frac{x}{2} \cos\left(\frac{6\pi x}{a}\right)\right) dx \\
 &= \frac{1}{a} \int_{-a/2}^{a/2} x dx + \frac{1}{a} \int_{-a/2}^{a/2} x \cos\left(\frac{6\pi x}{a}\right) dx \\
 &= I_1 + I_2.
 \end{aligned}$$

Now solve I_1 and I_2 separately we get,

$$\begin{aligned} I_1 &= \frac{1}{a} \int_{-a/2}^{a/2} x dx \\ &= \frac{1}{a} \left. \frac{x^2}{2} \right|_{-a/2}^{a/2} \\ &= \frac{1}{a} \left(\frac{a^2}{4} - \frac{a^2}{4} \right) \\ &= 0 \end{aligned}$$

$$I_2 = \frac{1}{a} \int_{-a/2}^{a/2} x \cos\left(\frac{6\pi x}{2}\right) dx$$

The product of an even function, $\cos(6\pi x/2)$ and an odd function x , is an odd function and the integration of an odd function results in zero. We immediately implies $I_2 = 0$.

We can also prove the same argument by solving it,

$$\begin{aligned} u &= x & dv &= \cos\left(\frac{6\pi x}{a}\right) \\ du &= dx & v &= \frac{\sin\left(\frac{6\pi x}{a}\right)}{6\pi/a} \end{aligned}$$

Integrating it by parts,

$$\begin{aligned} \int u v &= u v - \int v du \\ I_2 &= x \cdot \frac{\sin(6\pi x/2)}{6\pi/a} \Big|_{-a/2}^{a/2} - \int_{-a/2}^{a/2} \frac{\sin(6\pi x/2)}{6\pi/a} dx \\ &= \frac{a}{6\pi} \cdot x \sin(6\pi x/2) \Big|_{-a/2}^{a/2} - \frac{a}{6\pi} \int_{-a/2}^{a/2} \sin(6\pi x/2) dx \\ &= \frac{a}{6\pi} \left[\frac{a}{2} \sin(3\pi) - \frac{a}{2} \sin(-3\pi) \right] + \frac{a}{6\pi} \cdot \frac{\cos(6\pi x/2)}{6\pi/a} x \Big|_{-a/2}^{a/2} \\ &= \frac{a}{6\pi} (0) + \frac{a}{6\pi} \cdot \frac{a}{6\pi} (\cos(3\pi) - \cos(-3\pi)) \\ &= \frac{a^2}{12\pi^2} (-1 + 1) \\ &= 0 \end{aligned}$$

Therefore, the expectation value of position is

$$\bar{x} = I_1 + I_2 = 0.$$

b). The uncertainty in momentum is,

$$\begin{aligned}\langle p \rangle = \bar{p} &= \int_{-a/2}^{a/2} \psi_3^*(x) p \psi_3(x) dx \\ &= \frac{2}{a} \int_{-a/2}^{a/2} \cos\left(\frac{3\pi x}{a}\right) \cdot -i\hbar \frac{\partial}{\partial x} \cdot \cos\left(\frac{3\pi x}{a}\right) dx \\ &= \frac{2}{a} \int_{-a/2}^{a/2} \cos\left(\frac{3\pi x}{a}\right) \cdot -i\hbar \cdot \sin\left(\frac{3\pi x}{a}\right) \cdot \frac{3\pi}{a} dx \\ &= \frac{2}{a} \cdot -i\hbar \cdot \frac{3\pi}{a} \int_{-a/2}^{a/2} \cos\left(\frac{3\pi x}{a}\right) \cdot \sin\left(\frac{3\pi x}{a}\right) dx \\ &= 0\end{aligned}$$

because the product of an even function and an odd function is an odd function, the integration of an odd function results in zero. Above two results are expected from the symmetry of the potential and also from the fact that while taking the average, we consider both the positive and negative values. The positive values of x are equally likely as the negative x values. Similarly, the particle is free to move in either the +ive or -ive directions.

c). To calculate $\overline{x^2}$, we use the definition,

$$\begin{aligned}
 \langle x^2 \rangle = \overline{x^2} &= \int_{-a/2}^{a/2} \psi_3^*(x) x^2 \psi_3(x) dx \\
 &= \frac{2}{a} \int_{-a/2}^{a/2} x^2 \cos^2\left(\frac{3\pi x}{a}\right) dx \\
 &= \frac{2}{a} \int_{-a/2}^{a/2} x^2 \left(\frac{1 + \cos\left(\frac{2 \cdot 3\pi x}{a}\right)}{2} \right) dx \\
 &= \frac{2}{a} \int_{-a/2}^{a/2} \left(\frac{x^2}{2} + \frac{x^2 \cos\left(\frac{6\pi x}{a}\right)}{2} \right) dx \\
 &= \frac{1}{a} \int_{-a/2}^{a/2} x^2 dx + \frac{1}{a} \int_{-a/2}^{a/2} x^2 \cos\left(\frac{6\pi x}{a}\right) dx \\
 &= I_1 + I_2.
 \end{aligned}$$

Now,

$$\begin{aligned}
 I_1 &= \frac{1}{a} \int_{-a/2}^{a/2} x^2 dx \\
 &= \frac{1}{a} \left. \frac{x^3}{3} \right|_{-a/2}^{a/2} \\
 &= \frac{1}{3a} \left(\frac{a^3}{8} + \frac{a^3}{8} \right) \\
 &= \frac{1}{3a} \frac{2a^3}{8} \\
 I_1 &= \frac{a^2}{12}.
 \end{aligned}$$

$$I_2 = \frac{1}{a} \int_{-a/2}^{a/2} x^2 \cos\left(\frac{6\pi x}{a}\right) dx.$$

Let we suppose,

$$\begin{aligned}
 u &= x^2 & dv &= \cos\left(\frac{6\pi x}{a}\right) \\
 du &= 2x dx & v &= \frac{\sin\left(\frac{6\pi x}{a}\right)}{\frac{6\pi}{a}}
 \end{aligned}$$

Integrating it by parts,

$$\int u v = u v - \int v du$$

$$\begin{aligned}
 &= \frac{1}{a} \left[x^2 \frac{\sin\left(\frac{6\pi x}{a}\right)}{\frac{6\pi}{a}} \Big|_{-a/2}^{a/2} - \int_{-a/2}^{a/2} \frac{\sin\left(\frac{6\pi x}{a}\right)}{\frac{6\pi}{a}} 2x dx \right] \\
 &= \frac{1}{a} \left[0 - \frac{2a}{6\pi} \int_{-a/2}^{a/2} x \sin\left(\frac{6\pi x}{a}\right) dx \right] \\
 &= -\frac{2}{6\pi} \int_{-a/2}^{a/2} x \sin\left(\frac{6\pi x}{a}\right) dx \\
 &= -\frac{2}{6\pi} \left[x \frac{-\cos\frac{6\pi x}{a}}{6\pi/a} \Big|_{-a/2}^{a/2} - \int_{-a/2}^{a/2} \frac{-\cos\frac{6\pi x}{a}}{6\pi/a} dx \right] \\
 &= -\frac{2}{6\pi} \left[-\frac{a}{6\pi} \left(\frac{a}{2} \cos(3\pi) + \frac{a}{2} \cos(-3\pi) \right) + \frac{a}{6\pi} \frac{\sin\frac{6\pi x}{a}}{6\pi/a} \Big|_{-a/2}^{a/2} \right] \\
 &= -\frac{2}{6\pi} \left[-\frac{a}{6\pi} \left(\frac{a}{2} (-1) + \frac{a}{2} (-1) \right) + 0 \right] \\
 &= -\frac{2}{6\pi} \left[\left(-\frac{a}{6\pi} \right) (-a) \right] \\
 &= -\frac{2}{6\pi} \frac{a^2}{6\pi} \\
 I_2 &= -\frac{a^2}{18\pi^2}.
 \end{aligned}$$

Therefore,

$$\begin{aligned}
 \langle x^2 \rangle &= \bar{x^2} = I_1 + I_2 \\
 &= \frac{a^2}{12} - \frac{a^2}{18\pi^2} \\
 &= a^2 \left(\frac{1}{12} - \frac{1}{18\pi^2} \right) \\
 &= a^2 \left(\frac{1}{12} - 5.63 \times 10^{-3} \right) \\
 &= 0.077a^2.
 \end{aligned}$$

Even though $\langle x \rangle = 0$, the particle can be found anywhere inside the box, indicated by the non-zero value of $\langle x^2 \rangle$. This shows that the particle is traversing all values of x inside the box. If, by chance, both $\langle x \rangle = 0$ and $\langle x^2 \rangle = 0$, then,

$$\begin{aligned}
 (\Delta x)^2 &= \langle (x - \langle x \rangle)^2 \rangle \\
 &= \langle x^2 + \langle x \rangle^2 - 2x\langle x \rangle \rangle \\
 &= \langle x^2 \rangle + \langle x \rangle^2 \\
 &= 0,
 \end{aligned}$$

implying we would precisely know its position.

d). Further, we have to find $\langle p^2 \rangle$,

$$\begin{aligned}
 \langle p^2 \rangle &= \bar{p}^2 = \int_{-a/2}^{a/2} \psi_3^*(x) \hat{p}^2 \psi_3(x) dx \\
 &= \frac{2}{a} \int_{-a/2}^{a/2} \cos\left(\frac{3\pi x}{a}\right) (-i\hbar \frac{\partial}{\partial x}) (-i\hbar \frac{\partial}{\partial x}) \cos\left(\frac{3\pi x}{a}\right) dx \\
 &= \frac{2}{a} \int_{-a/2}^{a/2} \cos\left(\frac{3\pi x}{a}\right) \left(-\hbar^2 \frac{\partial}{\partial x} \left(-\sin\left(\frac{3\pi x}{a}\right) \frac{3\pi}{a} \right) \right) dx \\
 &= \frac{2\hbar^2}{a} \frac{3\pi}{a} \int_{-a/2}^{a/2} \cos\left(\frac{3\pi x}{a}\right) \frac{\partial}{\partial x} \left(\sin\left(\frac{3\pi x}{a}\right) \right) dx \\
 &= \frac{2\hbar^2}{a} \frac{3\pi}{a} \int_{-a/2}^{a/2} \cos\left(\frac{3\pi x}{a}\right) \cos\left(\frac{3\pi x}{a}\right) \left(\frac{3\pi}{a}\right) dx \\
 &= \frac{2\hbar^2}{a} \left(\frac{3\pi}{a}\right)^2 \int_{-a/2}^{a/2} \cos^2\left(\frac{3\pi x}{a}\right) dx \\
 &= \frac{2\hbar^2}{a} \left(\frac{3\pi}{a}\right)^2 \int_{-a/2}^{a/2} \left(\frac{1 + \cos\left(\frac{6\pi x}{a}\right)}{2} \right) dx \\
 &= \frac{2\hbar^2}{a} \left(\frac{3\pi}{a}\right)^2 \left[\frac{x}{2} \Big|_{-a/2}^{a/2} + \frac{\sin\left(\frac{6\pi x}{a}\right)}{2 \cdot \frac{6\pi}{a}} \Big|_{-a/2}^{a/2} \right] \\
 &= \frac{2\hbar^2}{a} \left(\frac{3\pi}{a}\right)^2 \left[\left(\frac{a/2}{2} - \frac{-a/2}{2} \right) + \frac{a}{12\pi} (\sin(3\pi) - \sin(-3\pi)) \right] \\
 &= \frac{2\hbar^2}{a} \left(\frac{3\pi}{a}\right)^2 \left[\frac{a}{4} + \frac{a}{4} \right] + 0 \\
 &= \frac{2\hbar^2}{a} \left(\frac{3\pi}{a}\right)^2 \left[\frac{a}{2} \right] \\
 &= \frac{2\hbar^2}{a} \left(\frac{9\pi^2}{a^2}\right) \frac{a}{2} \\
 &= \frac{9\pi^2 \hbar^2}{a^2} \\
 &= 88.7 \left(\frac{\hbar}{2}\right)^2
 \end{aligned}$$

Similar arguments will hold here, even though $\langle p \rangle = 0$, the momentum can have any value, indicated by the non-zero value of $\langle p^2 \rangle$. If, by chance, both $\langle p \rangle = 0$ and $\langle p^2 \rangle = 0$, then,

$$\begin{aligned}
 (\Delta p)^2 &= \langle (p - \langle p \rangle)^2 \rangle \\
 &= \langle p^2 + \langle p \rangle^2 - 2p\langle p \rangle \rangle \\
 &= \langle p^2 \rangle + \langle p \rangle^2 \\
 &= 0,
 \end{aligned}$$

implying we would precisely know the momentum of the particle.

As an aside, we can use the calculated values to verify the uncertainty principle,

$$\begin{aligned}\Delta x &= \sqrt{\langle (x - \langle x \rangle)^2 \rangle} \\ &= \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \\ &= \sqrt{\langle x^2 \rangle} \\ &= \sqrt{0.077a^2} \\ &= 0.27a.\end{aligned}$$

Similarly, the uncertainty in momentum is

$$\begin{aligned}\Delta p &= \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \\ &= \sqrt{\langle p^2 \rangle} \\ &= \sqrt{88.3 \left(\frac{\hbar}{a}\right)^2} \\ &= 9.39 \left(\frac{\hbar}{a}\right)\end{aligned}$$

The uncertainty in position times the uncertainty in momentum is,

$$\begin{aligned}\Delta x \cdot \Delta p &= 0.27a \times 9.39 \left(\frac{\hbar}{a}\right) \\ &= 2.5 \hbar, \quad \text{consistent with the uncertainty principle.}\end{aligned}$$

Answer 3.

(a)

In this problem, $A e^{ik_1x}$ represents the propagation of waves in the forward direction where $B e^{-ik_1x}$ represents backward motion. At nodes, according to the law of conservation of energy,

$$\begin{aligned}A^* A &= B^* B, & \text{which implies,} \\ B &= e^{i\phi} A\end{aligned}$$

This means that after reflecting from the barrier, the wave is moving in the backward

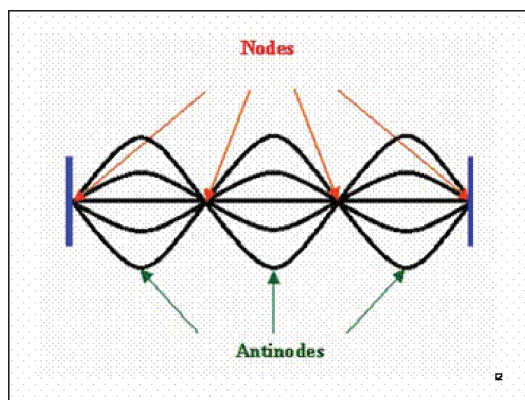
direction with some phase factor $e^{i\phi}$. So, for reflected wave,

$$\begin{aligned}
 \psi &= \left(A e^{ik_1x} + B e^{-ik_1x} \right) e^{-iEt/\hbar} \\
 &= \left(A e^{ik_1x} + A e^{i\phi} e^{-ik_1x} \right) e^{-iEt/\hbar} \\
 &= A e^{i\phi/2} \left[e^{ik_1x} e^{-i\phi/2} + e^{-i\phi/2} e^{-ik_1x} \right] e^{-iEt/\hbar} \\
 &= A e^{i\phi/2} \left[e^{i(k_1x - \phi/2)} + e^{-(ik_1x - \phi/2)} \right] e^{-iEt/\hbar} \\
 &= 2A e^{i\phi/2} \cos(k_1x - \phi/2) e^{-iEt/\hbar}
 \end{aligned}$$

This means, nodes occur only when,

$$\begin{aligned}
 k_1x - \phi/2 &= (2n + 1) \frac{\pi}{2} \\
 k_1x &= (2n + 1) \frac{\pi}{2} + \frac{\phi}{2} \\
 x_{\text{node}} &= (2n + 1) \frac{\pi}{2k} + \frac{\phi}{2k}, \quad \text{independent of time.}
 \end{aligned}$$

Hence Standing waves are produced, as shown in the figure.



Answer 4.

(a)

In the lowest energy state, $n = 1$, ψ has no nodes. Hence ψ_I must corresponds to $n = 2$, whereas ψ_{II} to $n = 3$. Further, since energy $E_n \propto n^2$ which implies $E_2 = 4$ eV. Therefore we get,

$$E_3 = 9 \text{ eV.}$$

b). By the same analysis, the lowest possible total energy for the particle in this system is,

$$E_0 = 1 \text{ eV}$$

Assignment 8: Spherical harmonics and the hydrogen atom

- (a) An electron is in the $2s$ orbital. At what point does the probability density $\Psi^*(r, \theta, \phi)\Psi(r, \theta, \phi)$ has its maximum value? Show that the density is maximum at the nucleus.

(b) The result from the previous part seems unphysical. Assume the nuclear diameter for it is 2×10^{-15} m. Calculate the total probability of finding the electron in the nucleus. You are allowed to use any assumptions in evaluating the integral.

(c) Calculate the position of the maxima in the radial probability distribution $P_r(r)$ for the $2s$ orbital. (In this part you would need access to a numerical or graphics package such as Matlab.)

- Use an analogy with the particle in the box to explain why the energy levels for the H atom are not equally spaced.

- Locate the radial and angular nodes in the H orbital $\psi_{3p_x}(r, \theta, \phi)$.

- In spherical coordinates, $z = r \cos \theta$. Calculate $\langle z \rangle$ for the H atom in the ground state. Without doing the calculations, what do you expect for $\langle x \rangle$ and why?

- As the principal quantum number n increases, the electron is more likely to be found far from the nucleus. It can be shown that for single-electron atoms and ions,

$$\langle r \rangle_{n,l} = \frac{n^2 a_o}{Z} \left[1 + \frac{1}{2} \left(1 - \frac{l(l+1)}{n^2} \right) \right]$$

Calculate the value of n for an s state in the H atom, such that $\langle r \rangle = 1000 a_o$. Round up to the nearest integer. What is the ionization energy of the H atom in this state in electron volts? Compare your answer with the ionization energy of the H atom in the ground state.

- Consider the probability of finding the electron in the hydrogen atom somewhere inside a cone of semiangle 23.5° of the $+z$ axis ("arctic polar region")

(a) If the electron were equally likely to be found anywhere in space, What would be the probability of finding the electron in the arctic polar region?

(b) Suppose the atom is in the state $n = 2, l = 1, m_l = 0$, recalculate the probability of finding the electron in the arctic polar region.

The hydrogen atom

Answer 1.

(a). For a 2s orbital, $n = 2$, $l = 0$, $m_l = 0$. Therefore, the wavefunction is,

$$\Psi_{2,0,0} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}$$

The probability density is,

$$\begin{aligned} p &= \Psi_{2,0,0}^* \Psi_{2,0,0} \\ &= \left(\frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}\right) \left(\frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}\right) \\ p &= \frac{1}{16(2\pi)} \left(\frac{Z}{a_0}\right)^3 \left(2 - \frac{Zr}{a_0}\right)^2 e^{-Zr/a_0}. \end{aligned}$$

It is evident from this expression that p is maximum when $r = 0$. This is quite unphysical as it suggests that the probability of finding the electron is maximum at the nucleus. This paradox is resolved by using the radial probability density instead of the probability density.

(b). To calculate the total probability of finding the electron within the nucleus, we integrate,

$$\begin{aligned} P &= \int_{Vol} \psi_{2,0,0}^* \psi_{2,0,0} dV \\ &= \int_{r=0}^{r_{\text{nucleus}}} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \frac{1}{16(2\pi)} \left(\frac{Z}{a_0}\right)^3 \left(2 - \frac{Zr}{a_0}\right)^2 e^{-Zr/a_0} r^2 \sin\theta d\theta d\phi dr \\ &\quad \text{since, } \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \sin\theta d\theta d\phi = 4\pi \\ &= \frac{4\pi}{32\pi} \left(\frac{Z}{a_0}\right)^3 \int_{r=0}^{r_{\text{nucleus}}} r^2 \left(2 - \frac{Zr}{a_0}\right)^2 e^{-Zr/a_0} dr. \end{aligned}$$

Since we want to find the probability within the nucleus, it is a reasonable assumption that $r_{\text{nucleus}} \ll a_0$ (first Bohr's radius).

For example, if we assume $r_{\text{nucleus}} \approx 0.1a_0$, then the factor $\left(2 - \frac{Zr}{a_0}\right)^2 e^{-Zr/a_0}$ is almost a constant number $\approx \left(2 - \frac{Zr_{\text{nucleus}}}{a_0}\right)^2 e^{-Zr_{\text{nucleus}}/a_0}$. Therefore,

$$\begin{aligned} P &\approx \frac{1}{8} \left(\frac{Z}{a_0}\right)^3 \left(2 - \frac{Zr_{\text{nucleus}}}{a_0}\right)^2 e^{-Zr_{\text{nucleus}}/a_0} \int_{r=0}^{r_{\text{nucleus}}} r^2 dr \\ &\approx \frac{1}{8} \left(\frac{Z}{a_0}\right)^3 \left(2 - \frac{Zr_{\text{nucleus}}}{a_0}\right)^2 e^{-Zr_{\text{nucleus}}/a_0} \frac{r_{\text{nucleus}}^3}{3}, \end{aligned}$$

Solution set 7: The hydrogen atom

since $r_{\text{nucleus}} \ll a_0$, the factor $r_{\text{nucleus}}/a_0 \approx 0$. Further, letting $Z = 1$,

$$\begin{aligned} P &\approx \frac{1}{8} \left(\frac{1}{a_0} \right)^3 (2)^2 e^0 \frac{r_{\text{nucleus}}^3}{3} \\ &\approx \frac{1}{6} \frac{(2 \times 10^{-15} \text{ m})^3}{(0.5 \times 10^{-10} \text{ m})^3} \\ P &\approx 1 \times 10^{-15}. \end{aligned}$$

This probability is extremely small and leads towards the conclusion that the total probability of finding the particle inside nucleus is negligible.

(c) Let $Z = 1$,

$$P_r(r) = 4\pi \frac{1}{16(2\pi)} \left(\frac{1}{a_0} \right)^3 \left(2 - \frac{r}{a_0} \right)^2 e^{-r/a_0} r^2$$

Ignoring the constants as it does not affect our calculations,

$$\begin{aligned} P_r(r) &= \left(2 - \frac{r}{a_0} \right)^2 r^2 e^{-r/a_0} \\ \frac{dP_r'(r)}{dr} &= 2 \left(2 - \frac{r}{a_0} \right) \left(-\frac{1}{a_0} \right) r^2 e^{-r/a_0} + 2 \left(2 - \frac{r}{a_0} \right)^2 r e^{-r/a_0} + \left(-\frac{1}{a_0} \right) \left(2 - \frac{r}{a_0} \right)^2 r^2 e^{-r/a_0} \\ &= \left(2 - \frac{r}{a_0} \right) r e^{-r/a_0} \left(\frac{-2}{a_0} r + 2 \left(2 - \frac{r}{a_0} \right) - \frac{r}{a_0} \right) \\ &= \left(2 - \frac{r}{a_0} \right) r e^{-r/a_0} \left(\frac{-3r}{a_0} + 4 - \frac{2r}{a_0} \right) \\ \Rightarrow \left(2 - \frac{r}{a_0} \right) r e^{-r/a_0} \left(4 - \frac{5r}{a_0} \right) &= 0 \\ \left(2 - \frac{r}{a_0} \right) r e^{-r/a_0} \left(4 - \frac{5r}{a_0} \right) &= 0 \end{aligned}$$

Hence the maxima exist at $r = 2a_0$ and $r = \frac{4}{5}a_0$. The minima are at $r = 0$ and $r = \infty$.

Answer 3.

(a). For ψ_{3p_x} in the hydrogen atom,

$$n = 3, l = 1, m_l = \pm 1,$$

such that the overall wavefunction is,

$$\begin{aligned} \psi_{3p_x} &= \frac{\psi_{3,1,1} + \psi_{3,1,-1}}{\sqrt{2}} \\ &= \frac{1}{\sqrt{2}} \left(\frac{1}{81\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \left(6 - \frac{Zr}{a_0} \right) \left(\frac{Zr}{a_0} \right) e^{-Zr/3a_0} \sin \theta \left(e^{i\phi} + e^{-i\phi} \right) \right) \\ &= \frac{2}{81\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \left(6 - \frac{Zr}{a_0} \right) \left(\frac{Zr}{a_0} \right) e^{-Zr/3a_0} \sin \theta \cos \phi. \end{aligned}$$

Solution set 7: The hydrogen atom

The radial nodes occur when the wavefunction is zero. Therefore, for the radial nodes,

$$\left(6 - \frac{r}{a_0}\right) \left(\frac{r}{a_0}\right) e^{-r/3a_0} = 0,$$

which implies that nodes occur when $r = 0$, $r = 6a_0$ or when $r \rightarrow \infty$.

The number of radial nodes can also be found out using the formula,

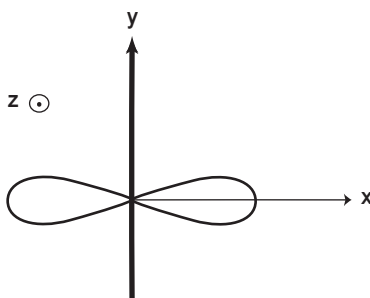
$$\begin{aligned} \text{Number of radial nodes} &= n - l - 1 \\ &= 3 - 1 - 1 \\ &= 1. \end{aligned}$$

Since $r = 0$ and $r \rightarrow \infty$ corresponds to the boundary conditions, the only possible radial node (excluding $r = 0$ and $r \rightarrow \infty$) is at $r = 6a_0$.

Similarly, for the angular nodes,

$$\sin \theta \cos \phi = 0,$$

which is possible only when $\theta = 0$ or $\phi = \pi/2$. The z -axis is one nodal axis and the yz plane is another nodal plane, as shown in the figure below. Since the z -axis is contained inside the yz plane, it is sufficient to say that the angular nodal plane is the yz plane.



Answer 4.

(a). For the hydrogen atom in ground state, $n = 1$, $l = 0$, $m_l = 0$, the corresponding normalized wavefunction is

$$\psi_{1,0,0} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}.$$

In spherical coordinates, the expectation value corresponding to $z = r \cos \theta$ is,

$$\begin{aligned}
 \langle z \rangle &= \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \psi^* z \psi dV \\
 &= \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \frac{1}{\pi} \left(\frac{1}{a_0} \right)^3 e^{-2r/a_0} (r \cos \theta) (r^2 \sin \theta d\theta d\phi dr) \\
 &= \frac{2\pi}{\pi} \left(\frac{1}{a_0} \right)^3 \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} r^3 e^{-2r/a_0} \cos \theta \sin \theta d\theta dr \\
 &= 2 \left(\frac{1}{a_0} \right)^3 \int_{r=0}^{\infty} r^3 e^{-2r/a_0} \frac{\sin^2 \theta}{2} \Big|_0^{\pi} dr \\
 &= 2 \left(\frac{1}{a_0} \right)^3 \int_{r=0}^{\infty} r^3 e^{-2r/a_0} (0 - 0) dr \\
 \langle z \rangle &= 0.
 \end{aligned}$$

Which shows that the expectation value is equal to zero.

(b). Similar argument will hold for $\langle x \rangle$ since there will be no preferred direction of orientation in space. This means all values of x , y , and z are equally likely due to spherical symmetry, and their average values $\langle x \rangle, \langle y \rangle$ and $\langle z \rangle$ are, each of them, identically zero.

Answer 5.

(a). Given is,

$$\langle r \rangle = \frac{n^2 a_0}{Z} \left[1 + \frac{1}{2} \left(1 - \frac{l(l+1)}{n^2} \right) \right].$$

For an s -state in the Hydrogen atom, $Z = 1$ and $l = 0$, therefore,

$$\begin{aligned}
 \langle r \rangle &= n^2 a_0 \left[1 + \frac{1}{2} \left(1 - \frac{0}{n^2} \right) \right] \\
 &= n^2 a_0 \left(1 + \frac{1}{2} \right) \\
 &= \frac{3}{2} n^2 a_0.
 \end{aligned}$$

But it is given that $\langle r \rangle = 1000 a_0$, therefore,

$$\begin{aligned}
 \frac{3}{2} n^2 a_0 &= 1000 a_0 \\
 n^2 &= \frac{2000}{3} \\
 n &= \sqrt{666} \\
 n &\approx 26.
 \end{aligned}$$

This will be the value of principle quantum number n for the given s state, which results in $\langle r \rangle = 1000a_0$.

(b). The ionization energy for the hydrogen atom is,

$$E_n = -\frac{13.6 \text{ eV}}{n^2}$$

Since $n = 26$ for our given s -state,

$$\begin{aligned} E_{26} &= -\frac{13.6}{26^2} \\ &= -0.02 \text{ eV}. \end{aligned}$$

The ionization energy is 0.02 eV, which is $0.02/13.6 = 0.1\%$ of the ground state ionization energy. This mean that for large values of n , only small amounts of energies are required to ionize the atom.

Answer 6.

(a). The probability of finding the electron at any radius in the arctic polar region is given by

$$\begin{aligned} P &= \frac{\left(\int r^2 R^* R dr \right) \left(\int \int_{\text{appropriate limits}} \Theta^*(\theta) \Theta(\theta) \Phi^*(\phi) \Phi(\phi) \sin \theta d\theta d\phi \right)}{\left(\int r^2 R^* R dr \right) \left(\int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \Theta^*(\theta) \Theta(\theta) \Phi^*(\phi) \Phi(\phi) \sin \theta d\theta d\phi \right)} \\ &= \frac{\left(\int \int_{\text{appropriate limits}} \Theta^*(\theta) \Theta(\theta) \Phi^*(\phi) \Phi(\phi) \sin \theta d\theta d\phi \right)}{\left(\int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \Theta^*(\theta) \Theta(\theta) \Phi^*(\phi) \Phi(\phi) \sin \theta d\theta d\phi \right)} \end{aligned}$$

For the sum of the upper and lower cone, the required probability is,

$$\begin{aligned} P &= \frac{2 \int_{\theta=0}^{\pi/8} \int_{\phi=0}^{2\pi} \sin \theta d\theta d\phi}{\int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \sin \theta d\theta d\phi} \\ &= \frac{2 \times 2\pi \int_{\theta=0}^{23.5} \sin \theta d\theta}{2\pi \int_{\theta=0}^{\pi} \sin \theta d\theta} \\ &= \frac{4\pi (-\cos \theta) \Big|_0^{23.5}}{2\pi (-\cos \theta) \Big|_0^{\pi}} \\ &= \frac{4\pi (-\cos (23.5) + \cos 0)}{2\pi (-\cos \pi + \cos 0)} \\ &= \frac{4\pi}{4\pi} (1 - \cos (23.5)) \\ P &= 0.08. \end{aligned}$$

(b). When the electron is in the state $n = 2, l = 1, m_l = 0$, then we exactly know the wavefunction,

$$\begin{aligned}\psi_{2,1,0} &= \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0} \cos \theta \\ &= \frac{1}{4\sqrt{2\pi}} a_0^{-5/2} r e^{-r/2a_0} \cos \theta.\end{aligned}$$

First (easy) method. Since we exactly know the wavefunction, the probability of locating the electron within the given angle, at any radius is given by,

$$\begin{aligned}P &= \frac{\left(\int r^2 R^* R dr\right) \left(\int \int_{\text{appropriate limits}} \Theta^*(\theta) \Theta(\theta) \Phi^*(\phi) \Phi(\phi) \sin \theta d\theta d\phi\right)}{\left(\int r^2 R^* R dr\right) \left(\int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \Theta^*(\theta) \Theta(\theta) \Phi^*(\phi) \Phi(\phi) \sin \theta d\theta d\phi\right)} \\ &= \frac{\left(\int \int_{\text{appropriate limits}} \Theta^*(\theta) \Theta(\theta) \Phi^*(\phi) \Phi(\phi) \sin \theta d\theta d\phi\right)}{\left(\int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \Theta^*(\theta) \Theta(\theta) \Phi^*(\phi) \Phi(\phi) \sin \theta d\theta d\phi\right)}\end{aligned}$$

For both the cones, the integrals becomes,

$$\begin{aligned}P &= \frac{\int_{\theta=0}^{\pi/8} \int_{\phi=0}^{2\pi} (\Theta_{1,0} \Phi_{1,0}) (\Theta_{1,0}^* \Phi_{1,0}^*) \sin \theta d\theta d\phi + \int_{\theta=\pi-\pi/8}^{\pi} \int_{\phi=0}^{2\pi} (\Theta_{1,0} \Phi_{1,0}) (\Theta_{1,0}^* \Phi_{1,0}^*) \sin \theta d\theta d\phi}{\int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (\Theta_{1,0} \Phi_{1,0})^2 \sin \theta d\theta d\phi} \\ &= \frac{2\pi \int_{\theta=0}^{23.5} \cos^2 \theta \sin \theta d\theta + 2\pi \int_{\theta=\pi-\pi/8}^{\pi} \cos^2 \theta \sin \theta d\theta}{2\pi \int_0^{\pi} \cos^2 \theta \sin \theta d\theta} \\ &= \frac{(2\pi)(-1) \frac{\cos^3 \theta}{3} \Big|_0^{23.5} + (2\pi)(-1) \frac{\cos^3 \theta}{3} \Big|_{\pi-\pi/8}^{\pi}}{(2\pi)(-1) \frac{\cos^3 \theta}{3} \Big|_0^{\pi}} \\ &= \frac{\frac{-2\pi}{3} [\cos^3 (23.5) - \cos^3 0 + \cos^3 \pi - \cos^3 (156.5)]}{\frac{-2\pi}{3} [\cos^3 \pi - \cos^3 0]} \\ &= \frac{[0.77 - 1 - 1 + 0.77]}{[-1 - 1]} \\ &= \frac{-0.45}{-2} \\ P &= 0.22,\end{aligned}$$

which is the required probability of finding the particle in the conical region.

Second (Difficult) method. Since the wavefunction is already normalized, the proba-

bility of finding the particle is simply equal to,

$$\begin{aligned}
 P &= \int_{vol} \psi^* \psi dV \\
 &= \int_{r=0}^{\infty} \int_{\theta=0}^{23.5} \int_{\phi=0}^{2\pi} \frac{1}{8(2\pi)} a_0^{-5} r^2 e^{-r/a_0} (\cos^2 \theta) r^2 \sin \theta d\phi d\theta dr \\
 &= \frac{a_0^{-5} (2\pi)}{8(2\pi)} \int_{r=0}^{\infty} \int_{\theta=0}^{23.5} r^4 e^{-r/a_0} \cos^2 \theta \sin \theta d\theta dr \\
 &= \frac{-a_0^{-5}}{8} \int_{r=0}^{\infty} r^4 e^{-r/a_0} \left. \frac{\cos^3 \theta}{3} \right|_0^{23.5} dr \\
 &= \frac{-a_0^{-5}}{24} \int_{r=0}^{\infty} r^4 e^{-r/a_0} (0.77 - 1) dr \\
 &= (9.5 \times 10^{-3})(-a_0^{-5}) \int_{r=0}^{\infty} r^4 e^{-r/a_0}
 \end{aligned}$$

Using the standard integral,

$$\int x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$$

$$P = (9.5 \times 10^{-3})(-a_0^{-5}) \frac{4!}{a_0^{-5}}$$

$$P = 0.24.$$

Assignment 9 (ungraded)**Part I: Multiple Choice Questions**

1. An experiment simultaneously measures the angular momentum components (L_x, L_y, L_z) of an electron with $l = 2$, when the field is consistently applied in the z direction. The experiment is repeated six times. Which of the following is physically a more realistic set of measurements of $(L_x, L_y, L_z)/\hbar$?
 - (A) $(1, 1, 2)$; $(1, 1, 2)$; $(1, 1, 2)$; $(1, 1, 2)$; $(1, 1, 2)$; $(1, 1, 2)$
 - (B) $(1, 1, 1)$; $(1, 1, -2)$; $(1, 1, -2)$; $(1, 1, 0)$; $(1, 1, 2)$; $(1, 1, 2)$
 - (C) $(1, -2, 1)$; $(2, 0, -2)$; $(-1, 2, -2)$; $(-2, -2, 0)$; $(1, 2, 2)$; $(2, 0, 2)$
 - (D) $(2.1, -0.76, 1)$; $(-0.35, 1.37, -2)$; $(-0.9, -1.19, -2)$; $(0.87, 1.30, 0)$;
 $(1.25, -0.67, 2)$; $(1.2, -0.74, 2)$
 - (E) $(2.1, -0.76, 0.23)$; $(-0.35, 1.37, -1.54)$; $(-0.9, -1.19, 1.32)$; $(0.87, 1.30, 0)$;
 $(1.25, -0.67, -0.67)$; $(1.2, -0.74, 0.19)$
2. A H atom is placed in vacuum, free of any external influences. This means we are completely ignorant of the m_l value. The average angular probability density $\Theta_{l,m_l}^* \Theta_{l,m_l} \Phi_{m_l}^* \Phi_{m_l}$ is,
 - (A) dependent on r , θ and ϕ
 - (B) dependent on θ and ϕ only
 - (C) dependent on θ only
 - (D) dependent on r only
 - (E) independent of r , θ and ϕ .

Part II: Short Questions

3. Write short answers to the following.
 - (a) What is the solution of the Schrodinger equation for $(n, l, m_l) = (2, 1, 1)$?

- (b) Argue that we cannot have an angular probability distribution that exists entirely in a plane?
- (c) The case $l = 0$ is a troubling one. How can an electron orbit the nucleus without possessing angular momentum?
- (d) What is meant by the normalization of a wavefunction? Explain in words.
- (e) Why is ψ , the wavefunction, an oscillatory function if $V(x) < E$?
- (f) Can a hydrogen atom absorb a photon whose energy exceeds its ionization energy, 13.6 eV?
- (g) Why is the wave nature not apparent to us in our daily lives?
- (h) Argue from the uncertainty principle that the lowest energy of an oscillator cannot be zero.

Part III: Not So Short Questions

4. What is the minimum angle the angular momentum vector may make with the z axis when $l = 3$?
5. A 200 kg satellite orbits the earth at a radius of 42,300 km and speed of 3.07 km/s. What might be its angular momentum quantum number? Is the angular momentum quantized for the satellite?
6. A hydrogen atom electron is in the $n = 2$ state with no knowledge of l or m_l . Calculate the probability that it would be found,
 - (a) in the region $z > 0$,
 - (b) within 30° of the xy plane, irrespective of the radius.
7. A hydrogen atom electron is in the $(n, l, m_l) = (2, 1, 1)$ orbital. The spherical harmonic function $\Theta_{1,1}(\theta)\Phi_1(\phi) = \sqrt{3/2} \sin \theta e^{i\phi}$ is defined so that,

$$\int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \Theta_{1,1}^*(\theta)\Theta_{1,1}(\theta)\Phi_1^*(\phi)\Phi_1(\phi) \sin \theta d\theta d\phi = 4\pi, \quad (1)$$

and the radial part of the wavefunction is $R_{2,1}(r) = \sqrt{1/(96\pi)}(1/a_0)^{3/2}(r/a_0)e^{-r/2a_0}$.

- (a) Calculate the probability that the electron would be found within 30° of the xy plane, irrespective of the radius.
- (b) How does one find the probability of locating the electron between $r = 2a_0$ and $r = 6a_0$, irrespective of the angle? Write the integral without solving it.

8. An electron in the H atom is in the $3d$ state,

$$\psi_{3,2,0} = \frac{1}{81\sqrt{6\pi}} \left(\frac{1}{a_0}\right)^{3/2} \frac{r^2}{a_0^2} e^{-r/3a_0} (3 \cos^2 \theta - 1). \quad (2)$$

What is the most probable radius at which to find the electron?

9. X-ray photons are emitted when electrons are suddenly decelerated. A 20 KeV electron emits **two** X-ray photons as it is brought to rest in two successive decelerations. The wavelength of the second photon is 1.30 \AA longer than the wavelength of the first.
- (a) What is the energy of the electron after the first deceleration?
- (b) What are the wavelengths of the emitted photons?
10. (a) The energy required to remove an electron from the sodium metal is 2.3 eV. Does sodium show the photoelectric effect for yellow light, with $\lambda = 589 \text{ nm}$? (b) What is the cutoff wavelength for photoelectric emission from sodium?
11. What accelerating voltage would be required for electrons in an electron microscope to obtain the same ultimate resolving power as that which could be obtained from from a “ γ -ray microscope” using 0.2 MeV γ rays? Use relativistic expression for the energy of the electron. (*HINT*: The resolving power is determined by the wavelength.)

Solutions to Short Questions 9

3. Write short answers to the following.

(a) What is the solution of the Schrodinger equation for $(n, l, m_l) = (2, 1, 1)$?

Ans. The solution is,

$$\psi_{2,1,1}(r, \theta, \phi) = \frac{1}{8\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} \left(\frac{r}{a_0}\right) e^{-r/2a_0} \sin \theta e^{i\phi}. \quad (1)$$

(b) Argue that we cannot have an angular probability distribution that exists entirely in a plane?

Ans. If the angular probability distribution is planar, the angular momentum will exist in a fixed direction, i.e., normal to the plane. For example, if the probability density exists in the xy plane, the angular momentum will deterministically point along $\pm z$ directions. This means that all three components of the angular momentum will be known, $L_x = L_y = 0$ as well as $L_z = \pm m_l \hbar$. But the uncertainty principle forbids us from knowing all three components of the angular momentum in one go. Therefore, the planar probability distribution is not allowed. Viewed from a different perspective, the conjugate variables L and θ will be precisely known, and this is not permissible.

(c) The case $l = 0$ is a troubling one. How can an electron orbit the nucleus without possessing angular momentum?

Ans. The angular momentum $L = \sqrt{l(l+1)}\hbar = 0$ when $l = 0$ (s -orbital). This means that the electron cannot be thought as a particle “orbiting” the nucleus. We must drop our classical perception of a moving electron in favour of a more faithful representation: a standing wave, called the orbital. In this mental picture, the electron exists everywhere the wavefunction is non-zero, it is smeared out in space and is present in all possible locations at the same time. Another possible response to this question might be that since $l = 0$ implies a spherically symmetric orbital, there is no preferred direction for the angular momentum to point to, hence it must be zero. Does $L = 0$ violate the uncertainty principle? No, it does not. Think about it!

(d) What is meant by the normalization of a wavefunction? Explain in words.

Ans. Normalization means that the particle exists somewhere. You go out looking for the particle in the entire universe, you will find it somewhere. Mathematically, the equivalent statement is that the probability of locating the particle somewhere is one, for it does exist. The act of normalizing a wavefunction computes this probability over the entire space and puts it equal to one.

(e) Why is ψ , the wavefunction, an oscillatory function if $V(x) < E$?

Ans. As $V(x) < E$, the particle is unbound, there are no restrictions on the energy value. From the Schrodinger equation, $d^2\psi/dx^2 = 2m/\hbar^2(V(x) - E)\psi$, the curvature $d^2\psi/dx^2$ and the wavefunction ψ have opposite signs: the wavefunction is concave towards the axis, resulting in oscillatory behaviour. Another way to look at it is by noticing that if ψ is non-oscillatory, it will asymptote to zero for certain values of x . However, this will restrict the particle in certain regions, which is not allowed since the particle is unbound.

(f) Can a hydrogen atom absorb a photon whose energy exceeds its ionization energy, 13.6 eV?

Ans. Yes, indeed it can. The hydrogen atom will then be ionized, the energy over and above 13.6 eV appears as the ejected electron's kinetic energy. Note that once you cross the ionization potential barrier, the absorbed photon or the ejected electron can have a continuous range of energies. Interestingly, sometimes, even if the absorbed photon's energy *slightly* exceeds 13.6 eV, electron ejection does not take place. Can you guess why? This is because of the non-zero reflectivity from a potential barrier which is a purely quantum mechanical phenomenon, as we have discussed in the Lectures on Tunneling!

(g) Why is the wave nature not apparent to us in our daily lives?

Ans. There are different equivalent answers to this question. First, the de Broglie relationship $\lambda = h/(mv)$ tells us that for massive objects and with the exceedingly small value of h , the wavelength is small compared to the resolution of our instrument, be it the eye, or the microscope. Hence, we cannot resolve the graininess of the wavelength and the wave picture is obscured. For revealing the wave picture, one has to go to small momenta (mv) making the wavelength

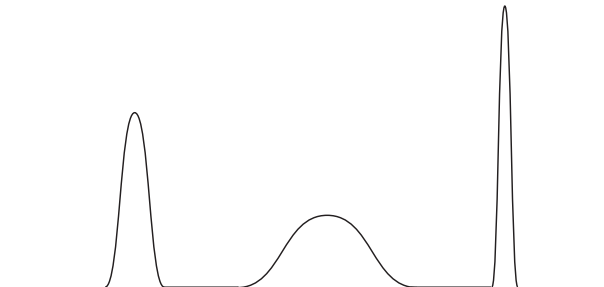
appreciably large so that our measuring apparatus can resolve the graininess.

- (h) Argue from the uncertainty principle that the lowest energy of an oscillator cannot be zero.

Ans. The lowest energy of an oscillator cannot be zero as this would mean that the momentum is precisely zero. But then the uncertainty in position must be of the order of infinity which is not possible for an oscillator (that is always bound) and has a restricted range of positions. Hence, there is always a zero point energy manifesting in interesting phenomena such as vacuum energy, the Casimir effect and the impossibility of achieving absolute zero temperature.

Final Examination: Modern Physics

1. The emission of a gas of Xe atoms is shown in the figure, with the brightness of the spectral line plotted with respect to the wavelength of the emission.

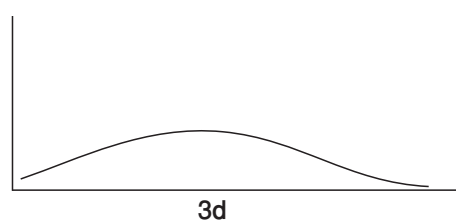
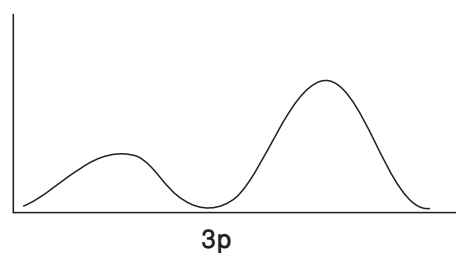
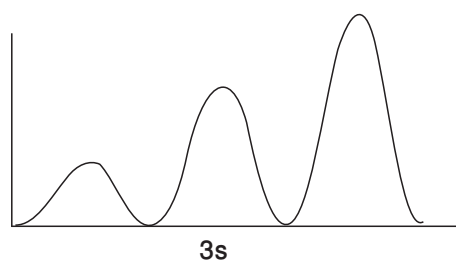


The spectral lines have different line widths because:

- A. The energy of the electrons in the Xe atom is not quantized.
 - B. The quantized energy levels have different lifetimes.
 - C. The spectrometer used for measuring the brightness has different sensitivities for different wavelengths.
 - D. Different atoms have different velocities resulting in varying Doppler broadening across the spectral lines.
 - E. Pressure variations inside the gas result in varying line width.
2. Consider a helium atom with atomic number $Z = 2$ and two electrons. The electrons are at distances \vec{r}_1 and \vec{r}_2 from the nucleus. The total electrostatic potential energy for the electrons is:

- A. $\frac{(-Ze)}{4\pi\epsilon_0} \frac{e}{r_1}$
- B. $\frac{(-Ze)}{4\pi\epsilon_0} \frac{e}{r_1} - \frac{(Ze)}{4\pi\epsilon_0} \frac{e}{r_2}$
- C. $\frac{(-Ze)}{4\pi\epsilon_0} \frac{e}{r_1} - \frac{(Ze)}{4\pi\epsilon_0} \frac{e}{r_2} + \frac{e^2}{4\pi\epsilon_0|\vec{r}_1 - \vec{r}_2|}$
- D. $\frac{(-Ze)}{4\pi\epsilon_0} \frac{e}{\sqrt{r_1^2 + r_2^2}}$
- E. $\frac{(-Ze)}{4\pi\epsilon_0} \frac{e}{r_1} - \frac{(Ze)}{4\pi\epsilon_0} \frac{e}{r_2} + \frac{(Ze)(Ze)}{4\pi\epsilon_0|\vec{r}_1 - \vec{r}_2|}$

3. The radial probability densities for the degenerate $n = 3$ states is shown in the figure. Now the K.E of an electron is the sum of a radial part and rotational part with the latter given by $L^2/2I$, I being the moment of inertia. The number of nodes decreases as l increases.



A possible reason for this is:

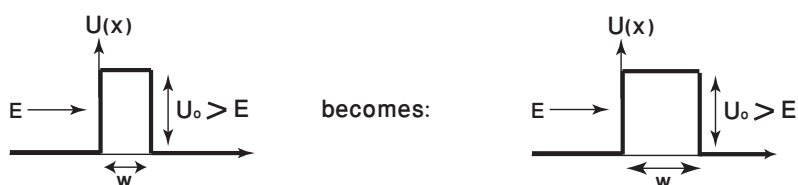
- A. Both the rotational and radial energies increase as l increases.
- B. The rotational energy increases but radial energy decreases as l increases. As the radial energy decreases, fewer nodes are expected.
- C. The rotational and radial energies remain constant for degenerate states.
- D. The total energy increases from $3s$ to $3p$ to $3d$ orbitals.
- E. None of the above.

4. An electron is known to exist in the $3p$ state in the hydrogen atom. Repeated measurements of the angular momentum yield:

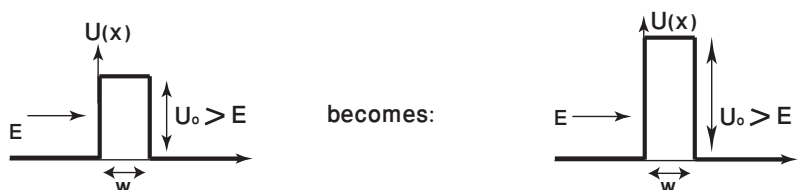
- A. $\sqrt{2} \hbar$ with a spread of $\pm \hbar$
- B. $\sqrt{2} \hbar$ with a spread of 0
- C. We cannot measure the angular momentum.
- D. $2 \hbar^2$ with a spread of $\pm \sqrt{2} \hbar$.
- E. 0 with a spread of $\pm \hbar$.

5. An electron is moving from left to right in a straight copper wire. It encounters a gap of width w in the wire. You would like to decrease the speed of the electron emerging from the right of the gap. Only possible way of achieving this is,

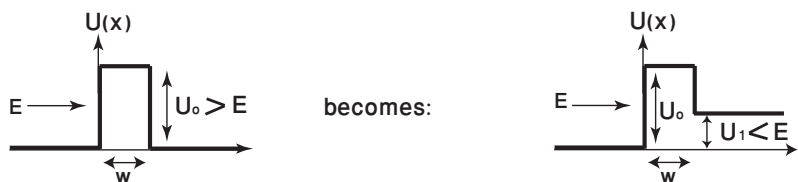
A. Increase the width w of the gap.



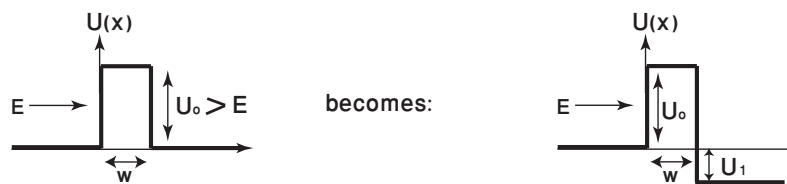
B. Increase U_0 , the potential energy of the gap .



C. Increase the potential energy to the right of the gap.



D. Decrease the potential energy to the right of the gap.



E. More than one of the changes above would decrease the speed of the electron.

6. Write brief answers to the following questions. (15 marks)

1. Mention one experimental evidence of the quantization of energy, of the uncertainty principle, and of the existence of orbitals.
2. For the H atom, what is the physical significance of the quantum numbers l and m_l ?
3. Show that the uncertainty in the momentum of a particle in an infinite well of width a for arbitrary n is $n\pi\hbar/a$.
4. An electron is trapped inside an infinite well. What is the expected value of its momentum? Is the particle at rest most of the times?
5. A particle is “thermal” if it is in equilibrium with its surroundings—its average kinetic energy would be $(3/2)k_B T$. Show that the wavelength of a thermal particle is,

$$\lambda = \frac{h}{\sqrt{3mk_B T}}.$$

7. A mosquito of mass 0.15 mg is found to be flying at a speed of 50 cm/s with an uncertainty of 0.5 mm/s. (a) How precisely may its position be known? (b) Does this inherent uncertainty present any hindrance to the application of classical mechanics?

(5 marks)

8. At what common energy E do the wavelengths of electrons and photons differ by a factor of 2? (5 marks)

9. Advance an argument that there is no bound(=quantized) state in a half-infinite well (shown in the diagram) unless the potential barrier V_0 is at least $h^2/(8ma^2)$. (*HINT*: What is the maximum possible wavelength inside the well?) (5 marks)

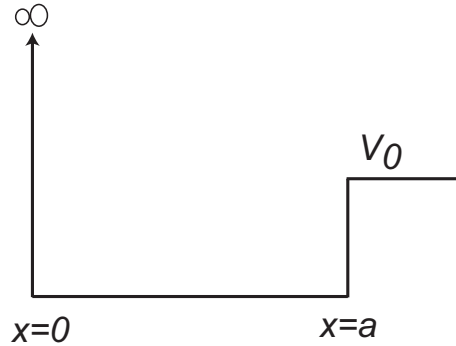


FIG. 1: Figure for Q 9.

10. The probability of transmission of a particle through a potential barrier (when $E < V_0$) is,

$$T = \frac{1}{1 + \sinh^2(k_2 a) \left(\frac{k_1^2 + k_2^2}{2k_1 k_2} \right)},$$

where the k 's and a have the usual meanings. What fraction of a beam of 50 eV electrons would get reflected from a 200 V, 1 nm wide electrostatic barrier? (5 marks)

11. For a given magnitude $L = \sqrt{l(l+1)}\hbar$ of \mathbf{L} , what are the largest and smallest values of L_z , and of L_x ? (5 marks)

12. A hydrogen atom electron is in the $(n, l, m_l) = (2, 1, 0)$ orbital. The spherical harmonic function $\Theta_{1,0}(\theta)\Phi_0(\phi) = \sqrt{3} \cos \theta$ is defined so that,

$$\int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \Theta_{1,0}^*(\theta)\Theta_{1,0}(\theta)\Phi_0^*(\phi)\Phi_0(\phi) \sin \theta d\theta d\phi = 4\pi,$$

and the radial part of the wavefunction is $R_{2,1}(r) = \sqrt{1/(96\pi)}(1/a_0)^{3/2}(r/a_0)e^{-r/2a_0}$.

1. Calculate the probability that the electron would be found within $\pm 60^\circ$ of the z axis.
2. How does one find the probability of locating the electron between $r = 2a_0$ and ∞ , irrespective of the angle? Write the integral without solving it. (10 marks)

13. Find the normalization constant A in the ground state ($1s$) of the hydrogen atom, $\psi_{1,0,0}(r, \theta, \phi) = A e^{-r/a_0}$, a_0 being the Bohr radius. Also find the expectation value of the potential energy for the ground state of hydrogen. Comment on your answer. **(10 marks)**

Final term solutions

Answer 1. B

Answer 2. C

Answer 3. B

Answer 4. B

Answer 5. C

Answer 6.

(6.1) Quantization of energy \Rightarrow Photoelectric effect, discrete energy levels and spectra, etc.
Uncertainty principle \Rightarrow Measurement of the position of an electron, single electron interference, natural broadening of spectral lines, etc.

Existence of orbitals \Rightarrow Bond formation in molecules.

(6.2) The azimuthal quantum number l with values $l = 0, 1, 2, \dots, (n - 1)$ determines the shape of the orbital. The orbitals with quantum number $l = 0, 1, 2,$ and 3 are called s, p, d and f orbitals, respectively. The magnetic quantum number m_l having values from $-l$ to $+l$ determines the orientation of orbitals in space in the presence of an external field.

(6.3) The energy of a particle in an infinite well of width a is,

$$E = \frac{n^2\pi^2\hbar^2}{2ma^2}.$$

Assume that for any arbitrary value of n , the uncertainty in the momentum of this particle is equal to momentum itself, so,

$$\begin{aligned} E &= \frac{p^2}{2m} \\ \Delta p &\approx p \\ &= \sqrt{2mE} \\ &= \sqrt{2m \frac{n^2\pi^2\hbar^2}{2ma^2}} \\ \Delta p &= \frac{n\pi\hbar}{a}. \end{aligned}$$

(6.4) For an infinite potential well, the momentum is either $+\sqrt{2mE}$ or it is $-\sqrt{2mE}$. Therefore, the expectation value of momentum, $\langle p \rangle$ is 0. For this case, either the particle is moving in forward direction or it is moving in backward direction. It will be never at rest.

(6.5) The average kinetic energy of a particle which is in thermal equilibrium with its surroundings is given by,

$$E = \frac{3}{2} k_B T.$$

The wavelength of this particle is,

$$\lambda = \frac{h}{p}.$$

The momentum is,

$$\begin{aligned} E &= \frac{p^2}{2m} \\ p &= \sqrt{2mE} \\ &= \sqrt{2m(3/2)k_B T} \\ p &= \sqrt{3mk_B T}. \end{aligned}$$

Hence, the wavelength is,

$$\lambda = \frac{h}{\sqrt{3mk_B T}}.$$

Answer 7. The uncertainty in position is given by the Heisenberg's uncertainty principle,

$$\begin{aligned} \Delta x \Delta p &\geq \frac{\hbar}{2} \\ \Delta x &\geq \frac{\hbar}{2\Delta p}. \end{aligned}$$

The uncertainty in momentum is,

$$\begin{aligned} \Delta p &= m\Delta v \\ &= (0.15 \times 10^{-6} \text{ Kg}) (5 \times 10^{-4} \text{ m/sec}) \\ &= 7.5 \times 10^{-11} \text{ Kg m/sec}. \end{aligned}$$

Therefore,

$$\begin{aligned} \Delta x &\geq \frac{1.054 \times 10^{-34} \text{ Kg m}^2/\text{sec}}{2 \times 7.5 \times 10^{-11} \text{ Kg m/sec}} \\ \Delta x &\geq 7 \times 10^{-25} \text{ m}. \end{aligned}$$

Since the uncertainty in position is extremely small on the classical scale, this presents no hindrance to the application of classical mechanics.

Answer 8. The energy of a photon is,

$$E = hf = \frac{hc}{\lambda_p}$$
$$E^2 = \frac{h^2c^2}{\lambda_p^2}.$$

The energy of an electron is (we must use the relativistic expression),

$$E^2 = p^2c^2 + m_0^2c^4$$
$$= \frac{h^2c^2}{\lambda_e^2} + m_0^2c^4.$$

We need to find out that common energy E at which the wavelength of electron and photon differ by a factor of 2. Therefore,

$$\frac{h^2c^2}{\lambda_p^2} = \frac{h^2c^2}{\lambda_e^2} + m_0^2c^4$$
$$\frac{1}{\lambda_p^2} = \frac{1}{\lambda_e^2} + \frac{m_0^2c^4}{h^2c^2}$$
$$\frac{1}{\lambda_p^2} = \frac{1}{\lambda_e^2} + \frac{m_0^2c^2}{h^2}.$$

For the common energy, the wavelength of electrons and photon differ by a factor of 2, i.e.,

$$\lambda_p = \lambda_e/2,$$

$$\frac{4}{\lambda_e^2} = \frac{1}{\lambda_e^2} + \frac{m_0^2c^2}{h^2}$$
$$\frac{3}{\lambda_e^2} = \frac{m_0^2c^2}{h^2}$$
$$\lambda_e^2 = \frac{3h^2}{m_0^2c^2}$$
$$\lambda_e = \sqrt{3} \left(\frac{h}{m_0c} \right).$$

The required common energy is,

$$E = \frac{hc}{\lambda_p} = \frac{2hc}{\lambda_e}$$
$$= \frac{2hc}{\sqrt{3}h} m_0c$$
$$= \frac{2}{\sqrt{3}} m_0c^2$$
$$E = 0.6 \text{ MeV}.$$

Answer 9.

For a half-infinite well potential, the energy E inside the well is directly proportional to k^2 , ($E = \hbar^2 k^2 / 2m$) and the wave number k is $k = 2\pi / \lambda$. Therefore, the maximum wavelength inside the well corresponds to the ground state energy. The maximum possible wavelength inside the well is simply equal to $2a$, such that,

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{2a} = \frac{\pi}{a}.$$

The energy inside the well is ,

$$\begin{aligned} E &= \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2}{2ma^2} = \frac{h^2 \pi^2}{8\pi^2 ma^2} \\ &= \frac{h^2}{8ma^2}. \end{aligned}$$

For the existence of bound states, it is necessary that $V_0 > E$. It implies that there will be no bound states until,

$$V_0 > \frac{h^2}{8ma^2},$$

which is the required result. Our well is semi-infinite, therefore our result is an upper bound, not necessarily the lowest bound.

Answer 10.

A barrier of 200 V represents an energy barrier of 200 eV to the electron. To find out the probability of transmission of a particle through a potential barrier (when $E < V_0$), first we need to calculate the k 's. i.e.,

$$\begin{aligned} k_1 &= \frac{\sqrt{2mE}}{\hbar} = \frac{\sqrt{2 \times 9.11 \times 10^{-31} \times 50}}{1.054 \times 10^{-34}} = 9.1 \times 10^{19} \text{ (Kg)}^{1/2} \text{ (eV)}^{1/2} \text{ (J.sec)}^{-1} \\ k_2 &= \frac{\sqrt{2m(V_0 - E)}}{\hbar} = \frac{\sqrt{2 \times 9.11 \times 10^{-31} \times (200 - 50)}}{1.054 \times 10^{-34}} = 1.5 \times 10^{20} \text{ (Kg)}^{1/2} \text{ (eV)}^{1/2} \text{ (J.sec)}^{-1}. \end{aligned}$$

By using these values,

$$\frac{k_1^2 + k_2^2}{2k_1 k_2} = 1.15.$$

Now, we need to be careful about the argument of \sinh because it should be a dimensionless quantity, i.e., a number, therefore,

$$\begin{aligned} k_2 a &= \frac{\sqrt{2 \times 9.11 \times 10^{-31} \text{ Kg} \times 150 \times 1.6 \times 10^{-19} \text{ J}}}{1.054 \times 10^{34} \text{ J.sec}} (1 \times 10^{-9} \text{ m}) \\ &= 62.7 \text{ (a number)}. \end{aligned}$$

We have converted now $V_0 - E = 150$ eV into its equivalent in Joules for dimensional consistency. Therefore, the transmission probability is,

$$\begin{aligned} T &= \frac{1}{1 + \sinh^2(k_2 a) \left(\frac{k_1^2 + k_2^2}{2k_1 k_2} \right)} \\ &= \frac{1}{1 + \sinh^2(62.7)(1.15)} \\ &= 1 \times 10^{-54} \approx 0 \end{aligned}$$

Therefore, $R = 1 - 10^{-54} \approx 1$, there will be almost total reflection.

Answer 11. For a given magnitude $L = \sqrt{l(l+1)} \hbar$ of L , the maximum value of L_z is $l\hbar$ and smallest value is $-l\hbar$ (considering the sign) and 0 (considering the magnitude). For L_x , the largest value is $\sqrt{l(l+1)} \hbar$ and the smallest value is $-\sqrt{l(l+1)} \hbar$ (considering the sign) and 0 (considering the magnitude).

Answer 12.

Since we exactly know the wavefunction, the probability of locating the electron within the given angle, at any radius is given by,

$$\begin{aligned} P &= \frac{\left(\int r^2 R^* R dr \right) \left(\int \int_{\text{appropriate limits}} \Theta^*(\theta) \Theta(\theta) \Phi^*(\phi) \Phi(\phi) \sin \theta d\theta d\phi \right)}{\left(\int r^2 R^* R dr \right) \left(\int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \Theta^*(\theta) \Theta(\theta) \Phi^*(\phi) \Phi(\phi) \sin \theta d\theta d\phi \right)} \\ &= \frac{\left(\int \int_{\text{appropriate limits}} \Theta^*(\theta) \Theta(\theta) \Phi^*(\phi) \Phi(\phi) \sin \theta d\theta d\phi \right)}{\left(\int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \Theta^*(\theta) \Theta(\theta) \Phi^*(\phi) \Phi(\phi) \sin \theta d\theta d\phi \right)}. \end{aligned}$$

It is given that $\Theta_{1,0}(\theta) \Phi_0(\phi) = \sqrt{3} \cos(\theta)$, hence for the area of both the inside polar cones, the integral becomes,

$$\begin{aligned}
 P &= \frac{\int_{\theta=0}^{\pi/3} \int_{\phi=0}^{2\pi} (\Theta_{1,0}^* \Phi_{1,0}^*) (\Theta_{1,0} \Phi_{1,0}) \sin \theta \, d\theta \, d\phi + \int_{\theta=\pi-\pi/3}^{\pi} \int_{\phi=0}^{2\pi} (\Theta_{1,0}^* \Phi_{1,0}^*) (\Theta_{1,0} \Phi_{1,0}) \sin \theta \, d\theta \, d\phi}{\int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (\Theta_{1,0} \Phi_{1,0})^2 \sin \theta \, d\theta \, d\phi} \\
 &= \frac{2\pi(3) \int_{\theta=0}^{\pi/3} \cos^2 \theta \sin \theta \, d\theta + 2\pi(3) \int_{\theta=\pi-\pi/3}^{\pi} \cos^2 \theta \sin \theta \, d\theta}{2\pi(3) \int_0^{\pi} \cos^2 \theta \sin \theta \, d\theta} \\
 &= \frac{(-1) \frac{\cos^3 \theta}{3} \Big|_0^{\pi/3} + (-1) \frac{\cos^3 \theta}{3} \Big|_{\pi-\pi/3}^{\pi}}{(-1) \frac{\cos^3 \theta}{3} \Big|_0^{\pi}} \\
 &= \frac{\frac{-1}{3} [\cos^3(\pi/3) - \cos^3(0) + \cos^3(\pi) - \cos^3(\pi - \pi/3)]}{\frac{-1}{3} [\cos^3 \pi - \cos^3 0]} \\
 &= \frac{[0.125 - 1 - 1 + 0.125]}{[-1 - 1]} \\
 &= \frac{-1.75}{-2} \\
 P &= 0.87,
 \end{aligned}$$

which is the required probability of finding the particle within $\pm 60^\circ$ of the z-axis.

Part(b). The probability of locating the electron between $r = 2a_0$ and ∞ , irrespective of the angle, is given by,

$$P = \frac{\int_{r=2a_0}^{\infty} 4\pi r^2 R^* R \, dr}{\int_{r=0}^{\infty} 4\pi r^2 R^* R \, dr}.$$

The denominator is equal to 1 and it is given that, $R_{2,1}(r) = \sqrt{1/96\pi}(1/a_0)^{3/2} (r/a_0)e^{-r/2a_0}$, therefore,

$$\begin{aligned}
 P &= \int_{r=2a_0}^{\infty} 4\pi r^2 R^* R \, dr \\
 &= 4\pi \left(\frac{1}{96\pi}\right) \left(\frac{1}{a_0}\right)^3 \int_{r=2a_0}^{\infty} \left(\frac{r}{a_0}\right)^2 e^{-r/a_0} r^2 \, dr.
 \end{aligned}$$

This integral will give us the probability of finding the electron between $r = 2a_0$ and ∞ .

Answer 13.

According to the normalization condition,

$$\begin{aligned}
 \int \int \int_{Volume} \psi^*(r, \theta, \phi) \psi(r, \theta, \phi) dV &= 1 \\
 \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} (A e^{-r/a_0}) (A e^{-r/a_0}) r^2 \sin \theta dr d\theta d\phi &= 1 \\
 \int_{r=0}^{\infty} A^2 e^{-2r/a_0} (4 \pi r^2) dr &= 1 \\
 4\pi A^2 \int_{r=0}^{\infty} e^{-2r/a_0} dr &= 1 \\
 4\pi A^2 \left[\frac{r^2 e^{-2r/a_0}}{(-2/a_0)} \Big|_0^{\infty} - \int_0^{\infty} 2r \frac{e^{-2r/a_0}}{(-2/a_0)} dr \right] &= 1
 \end{aligned}$$

Using the fact that $e^{-\infty} = 0$, we get

$$\begin{aligned}
 4\pi A^2 \left[(0 - 0) + a_0 \int_0^{\infty} r e^{-2r/a_0} dr \right] &= 1 \\
 4\pi A^2 a_0 \int_0^{\infty} r e^{-2r/a_0} dr &= 1 \\
 4\pi A^2 a_0 \left[\frac{r e^{-2r/a_0}}{(-2/a_0)} \Big|_0^{\infty} - \int_0^{\infty} \frac{e^{-2r/a_0}}{(-2/a_0)} dr \right] &= 1 \\
 4\pi A^2 a_0 \left[(0 - 0) + \frac{a_0}{2} \int_0^{\infty} e^{-2r/a_0} dr \right] &= 1 \\
 4\pi A^2 \left(\frac{a_0^2}{2} \right) \int_0^{\infty} e^{-2r/a_0} dr &= 1 \\
 4\pi A^2 \left(\frac{a_0^2}{2} \right) \left[\frac{e^{-2r/a_0}}{(-2/a_0)} \Big|_0^{\infty} \right] &= 1 \\
 4\pi A^2 \left(\frac{a_0^2}{2} \right) \left(\frac{-a_0}{2} \right) (e^{-\infty} - e^0) &= 1 \\
 4\pi A^2 \left(\frac{-a_0^3}{4} \right) (0 - 1) &= 1 \\
 4\pi A^2 \left(\frac{a_0^3}{4} \right) &= 1 \\
 A^2 &= \frac{1}{\pi a_0^3} \\
 A &= \frac{1}{\sqrt{\pi a_0^3}}.
 \end{aligned}$$

Therefore, the normalized wavefunction is,

$$\psi = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}.$$

To find out the expectation value of potential energy for the ground state of hydrogen atom,

we use the expression, $V = -e^2/4\pi\epsilon_0r$. So, by definition, the expectation value is,

$$\begin{aligned}\langle V \rangle &= \int \int \int_{Volume} \psi^* V \psi dV \\ &= \int_r \int_\theta \int_\phi \left(\frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \right) \left(-\frac{e^2}{4\pi\epsilon_0r} \right) \left(\frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \right) r^2 \sin\theta d\theta d\phi dr \\ &= \int_{r=0}^{\infty} \left(\frac{1}{\pi a_0^3} \right) \left(-\frac{e^2}{4\pi\epsilon_0r} \right) (4\pi r^2) e^{-2r/a_0} dr \\ &= \left(\frac{-e^2}{\pi \epsilon_0 a_0^3} \right) \int_{r=0}^{\infty} r e^{-2r/a_0} dr \\ \langle V \rangle &= \left(\frac{-e^2}{\pi \epsilon_0 a_0^3} \right) I_1,\end{aligned}$$

$$\begin{aligned}I_1 &= \int_{r=0}^{\infty} r e^{-2r/a_0} dr \\ &= \left. \frac{r e^{-2r/a_0}}{(-2/a_0)} \right|_0^{\infty} - \int_{r=0}^{\infty} \frac{e^{-2r/a_0}}{(-2/a_0)} dr \\ &= \frac{-a_0}{2} (0 - 0) + \frac{a_0}{2} \left. \frac{e^{-2r/a_0}}{(-2/a_0)} \right|_0^{\infty} \\ &= \left(\frac{a_0}{2} \right) \left(-\frac{a_0}{2} \right) (e^{-\infty} - e^0) \\ &= -\left(\frac{a_0^2}{4} \right) (-1) \\ I_1 &= \frac{a_0^2}{4}.\end{aligned}$$

Therefore, the expectation value or potential energy is,

$$\begin{aligned}&= \left(\frac{-e^2}{\pi \epsilon_0 a_0^3} \right) \left(\frac{a_0^2}{4} \right) \\ \langle V \rangle &= -\frac{e^2}{4 \pi \epsilon_0 a_0}.\end{aligned}$$

The shows that the expected (average) value of the potential energy is the same as if there is an electron at distance a_0 from the nucleus. This is expected from Bohr's model. The expectation value coming from a quantum calculation yields the same result as is expected from the classical theory.