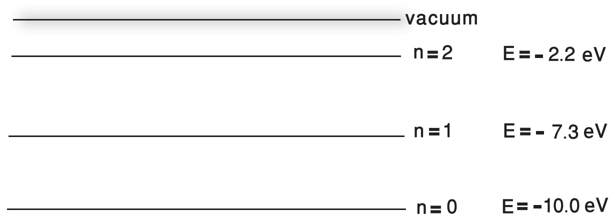
Assignment 4: Uncertainty principle, Bohr's model, Sommerfeld's quantization

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 (^{1}H) is 13.6 eV. What is the ionization energy of tritium (^{3}H)?

3. A hydrogen atom in the ground state absorbs a 30.0 eV photon. What is the speed of the librated 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,

$$E = \frac{n^2\,\hbar^2}{2I} \qquad\qquad n = 0, 1, 2, 3, \ldots, \tag{1}$$

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 it 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!

PH-102 **Solution Set # 4** October, 5, 2009

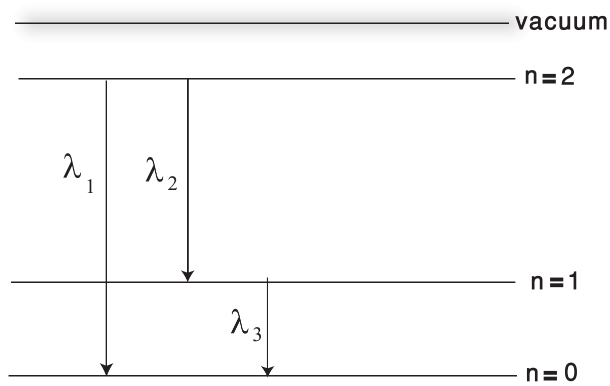
Uncertainty principle, Bohr's model, Sommerfeld's quantization

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,

$$\begin{aligned} n = 2 &\longrightarrow n = 0 \\ n = 2 &\longrightarrow n = 1 \\ n = 1 &\longrightarrow n = 0\,. \end{aligned}$$



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,

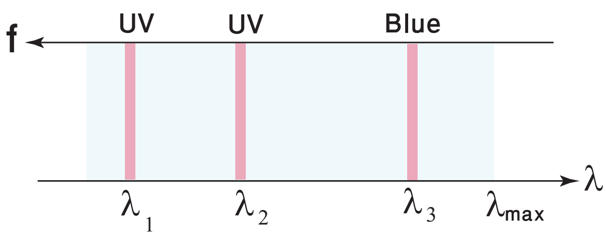
$$\begin{aligned} \Delta E &= hf \\ &= \frac{hc}{\lambda} \\ \lambda &= \frac{hc}{\Delta E}. \end{aligned}$$

Therefore, the wavelengths will be,

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

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

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



Now, there will be a maximum wavelength which corresponds to the energy difference between vacuum and the immediate lower state ($n = 2$).

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

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 $10\,\mathrm{eV}$, therefore, gamma rays will always ionize the atom, freeing the electrons into vacuum.

(d)

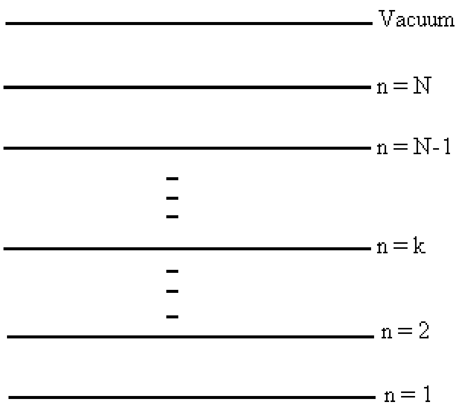
The brightness of the spectral lines depends upon the number of photons contributing to the emission lines. The number of photons emitted depends upon the number of electrons that jump from the higher to lower energy levels. However, all levels are not equally populated to start off with. The lower energy 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.



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

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,

$$\begin{aligned} v &= \sqrt{\frac{2(16.4)\,\text{eV}}{m}} \\ &= \sqrt{\frac{2\ (16.4)\,1.6\times10^{-19}\ \text{Kg}\,\text{m}^2/\text{s}^2}{9.11\times10^{-31}\ \text{Kg}}} \\ &= \sqrt{5.76\times10^{12}\ \text{m}^2/\text{sec}^2} \\ &= 2.4\times10^{6}\ \text{m/sec}\,. \end{aligned}$$

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,

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

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 $p \sim \hbar/(2\,r)$ 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,

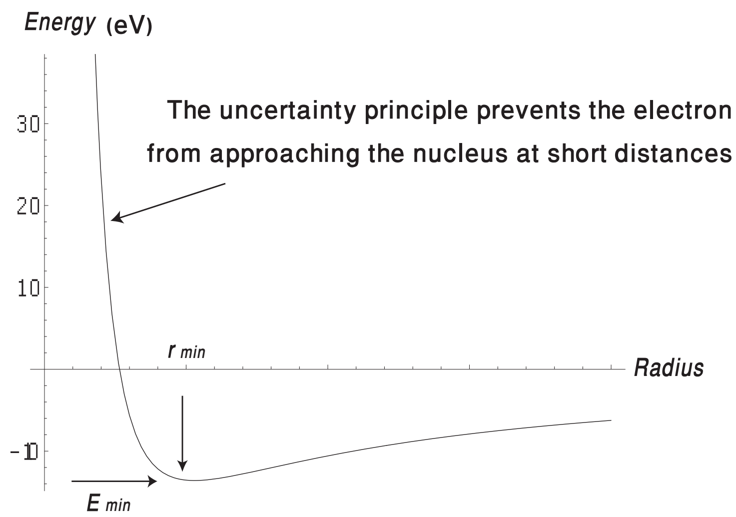
$$\begin{aligned}\text{Total Energy} &= E = K.E + P.E \\ &= \frac{\hbar^2}{2mr^2} - \frac{Ze^2}{4\pi\epsilon_o r}.\end{aligned}$$

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

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

Setting this equal to zero,

$$\begin{aligned}\frac{-\hbar^2}{mr^3_{min}} + \frac{Ze^2}{4\pi\epsilon_o r^2_{min}} &= 0 \\ \frac{Ze^2}{4\pi\epsilon_o r^2_{min}} &= \frac{\hbar^2}{mr^3_{min}} \\ r_{min} &= \frac{4\pi\epsilon_o\hbar^2}{mZe^2}. \\ &= 0.53\ \mathring{A},\end{aligned}$$



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,

$$\begin{aligned} \text{Total Energy} &= E = K.E + P.E \\ &= \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\epsilon_o r}. \end{aligned} \tag{1}$$

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

$$\begin{aligned} \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\epsilon_o r} &= 0 \\ \frac{\hbar^2}{2mr^2} &= \frac{4\pi\epsilon_o r}{e^2} \\ r_{ion} = \frac{2\pi\epsilon_o\hbar^2}{me^2} &= 0.24\,\text{Å}. \end{aligned}$$

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,

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

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),

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

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

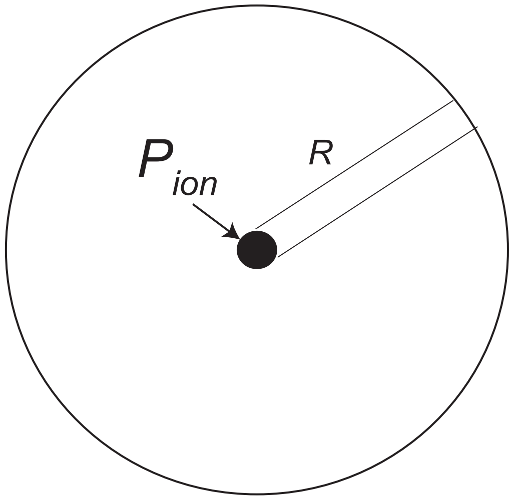
$$\left.\frac{\partial E}{\partial r}\right|_{r=r_{ion}} = \frac{-\hbar^2}{m}\left(\frac{1}{r_{ion}}\right)^3 + \frac{e^2}{4\pi\epsilon_o}\left(\frac{1}{r_{ion}}\right)^2 = -3.9\times 10^7\,\mathrm{J\,m^{-1}},$$

resulting in the ionizing pressure,

$$\begin{aligned} P_{ion} &= -\frac{\partial E}{\partial r}\,\frac{1}{4\pi r_{ion}^2} \\ &= 5.2\times 10^{13}\,\mathrm{Pa}. \end{aligned}$$

(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,

$$\rho = \frac{m_p}{\frac{4}{3}\pi r_{ion}^3} = 2.8 \times 10^4 \text{ kg m}^{-3}. \tag{2}$$

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,

$$\begin{aligned} P_{ion} &= \rho\, g\, R = \frac{\rho\, G\, M}{R} \qquad (3) \\ \implies R &= \frac{\rho G M}{P_{ion}} = 3.5 \times 10^{-20}\, M \text{ m}. \qquad (4) \end{aligned}$$

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

$$\begin{aligned} \rho = 2.8 \times 10^4 \text{ kg m}^{-3} &= \frac{M}{\frac{4}{3}\pi R^3} \qquad (5) \\ \implies M &= \frac{4}{3}\,\pi \rho R^3. \qquad (6) \end{aligned}$$

Inserting the value of M into (4) and then back substituting results in,

$$\begin{aligned} M &= 4 \times 10^{26} \text{ kg}, \\ R &= 1.6 \times 10^{7} \text{ m}. \end{aligned}$$

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

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.

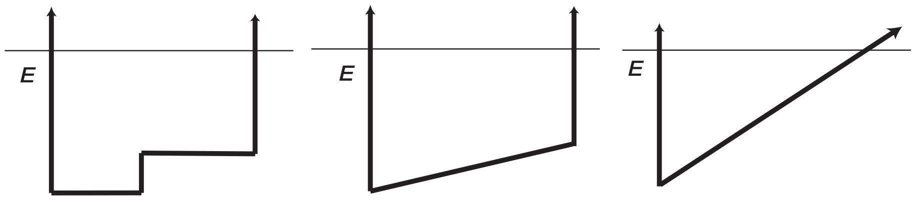


FIG. 1: Figure for Question 1.

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 $n \to \infty$? 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,

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

   where k_2 is the wavenumber inside the well.

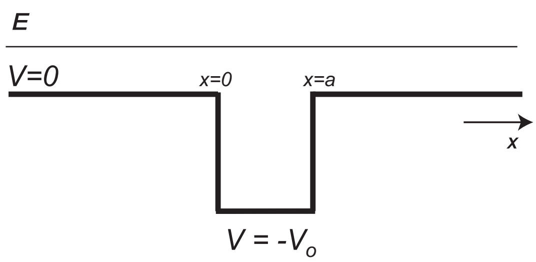


FIG. 2: Figure for Question 3.

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

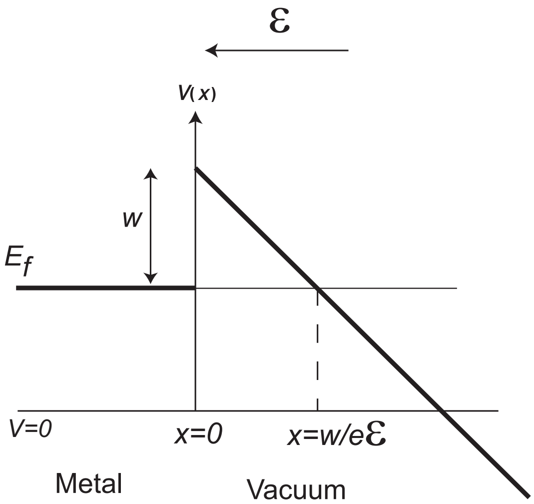
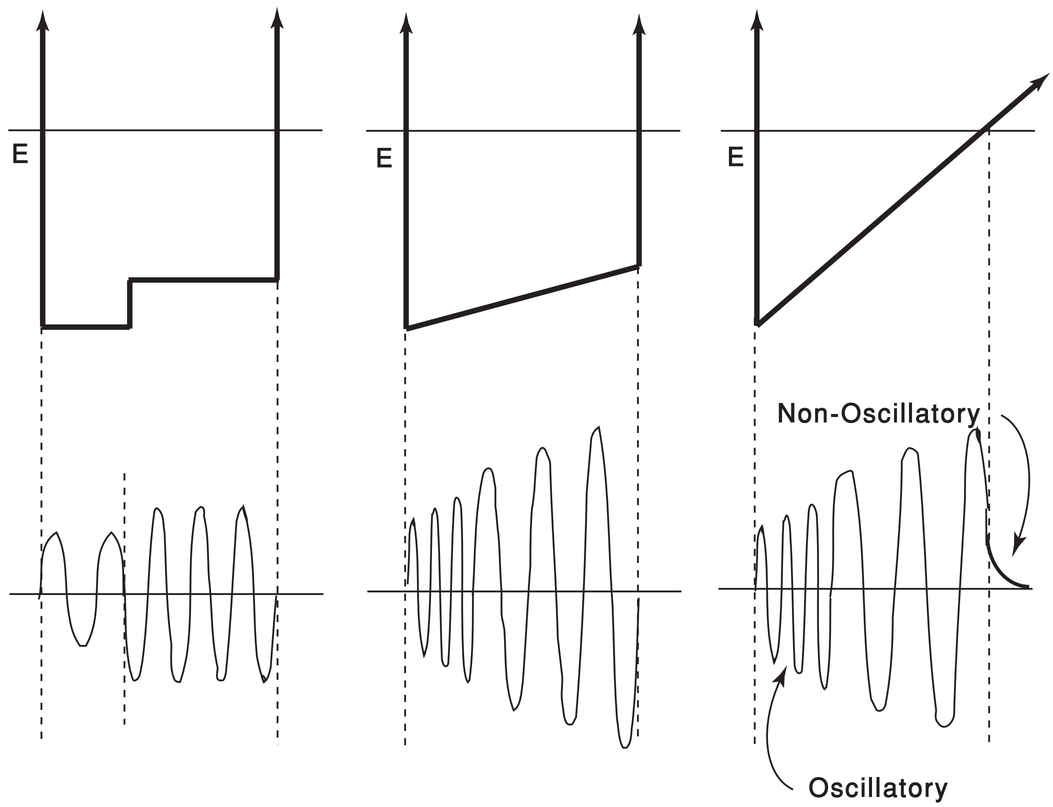


FIG. 3: Figure for Question 4.

PH-102 **Solution Set # 6** November, 24, 2009

Potential Steps, Barriers and Wells

Answer 1.



Answer 2.

(a)

As the potential energy of the particle is zero within the well, its total quantized energy equals its kinetic energy,

$$
\begin{aligned}
E &= \frac{\pi^2\hbar^2 n^2}{2ma^2} \qquad (1)\\
E &= 2.1\,\mathrm{MeV}\,.
\end{aligned}
$$

(b)

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

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

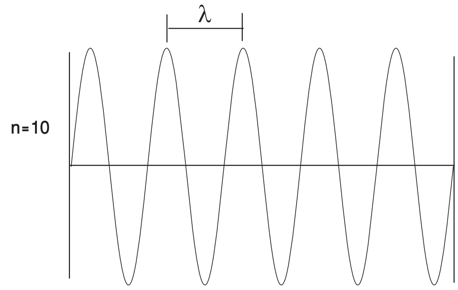
Therefore, the uncertainty in momentum will be of the order of p and we can say, $\Delta p \approx p$.

(c)

To findout the uncertainty in position, we use the uncertainty principle,

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

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



Since the momentum inside the well is given by,

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

Substituting the value of E from equation (1), we get,

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

The uncertainty in position will become,

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

(d) Since,

$$\begin{aligned}\Delta p = p &= \frac{\pi \hbar n}{a} = 2.5 \times 10^{-23}\,\mathrm{Kg\,m/sec} \\ \Delta x &= \frac{a}{\pi n} = 4.2 \times 10^{-12}\,\mathrm{m}\,.\end{aligned}$$

When $n \to \infty$, we can conclude that,

$$\Delta p \to \infty, \qquad \text{such that,} \qquad \Delta x \to 0\,.$$

Which means that the we can precisely find the position of the particle at any location, which is consistent with classical results. High n states correspond to the classical scenario. From equation (1), it is clear that high n leads to large energies correspond to the ground state energy. This is what classically observed.

Answer 3.

(a)

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

$$\psi(x) = \begin{cases} \psi_1(x) = A\,e^{(ik_1 x)} + B\,e^{(-ik_1 x)} & x \leq 0 \\ \psi_2(x) = C\,e^{(ik_2 x)} + D\,e^{(-ik_2 x)} & 0 < x < a \\ \psi_3(x) = E\,e^{(ik_2 x)} & x \geq a \end{cases}$$

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 $x = 0$,

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

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,

$$\begin{aligned} A + B &= C + D & (2) \\ ik_1(A - B) &= ik_2(C - D) & (3) \\ Ce^{ik_2a} + De^{-ik_2a} &= Ee^{ik_1a} & (4) \\ ik_2(Ce^{ik_2a} - De^{-ik_2a}) &= ik_1(Ee^{ik_1a})\,. & (5) \end{aligned}$$

Equation (3) can also be written as,

$$A - B = \frac{k_2}{k_1}\,(C - D)\,. \tag{6}$$

Adding equation (2) and (6), we get,

$$2A = (C + D) + \frac{k_2}{k_1}(C - D). \tag{7}$$

Similarly, equation (5) can be written as,

$$Ce^{ik_2a} - De^{-ik_2a} \;=\; \frac{k_1}{k_2}Ee^{ik_1a}. \tag{8}$$

Adding equation (3) and (8), we get

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

subtracting equation (3) and (8) yields,

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

substitute values of C and D in equation (7), we get,

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

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,

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

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 $k_2 = \frac{\sqrt{2m(E+V_o)}}{\hbar}$, substituting values into the denominator,

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

Therefore, transmissivity is,

$$
\begin{aligned}
T &= \frac{1}{1+\frac{1}{4}\left(\frac{-V_0}{\sqrt{E(E+V_0)}}\right)^2\sin^2(k_2a)} \\
&= \frac{1}{1+\frac{1}{4}\left(\frac{V_0^2}{E(E+V_0)}\right)\sin^2(k_2a)} \\
\frac{1}{T} &= 1+\frac{1}{4}\left(\frac{V_0^2}{E(E+V_0)}\right)\sin^2(k_2a)\,,
\end{aligned}
$$

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, $a \simeq 0.5$Å, substitute values,

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

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.

Furthur, 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 $c = w + E_f$,

$$\begin{aligned} y &= mx + c \\ V(x) &= -e\,\varepsilon x + w + E_f \\ V(x) - E_f &= w - e\,\varepsilon x\,. \end{aligned}$$

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,

$$\begin{aligned} u &= w - e\,\varepsilon\, x \\ du &= -e\,\varepsilon\, dx \\ dx &= \frac{-1}{e\,\varepsilon}\, dx, \end{aligned}$$

$$\begin{aligned} &\text{when } x = 0, && u = w, \quad \text{and} \\ &\text{when } x = w/e\,\varepsilon, && u = 0\,. \end{aligned}$$

Hence, the integration reduces to,

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

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

(d)

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

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

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

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

Recitation on infinite well

1. An electron is confined in an infinite well of 30 cm width.

   (a) What is the ground-state energy?

   (b) In this state, what is the probability that the electron would be found within 10 cm of the left-hand wall?

   (c) If the electron instead has an energy of 1.0 eV, what is the probability that it would be found within 10 cm of the left-hand wall?

   (d) For the 1-eV electron, what is the distance between nodes and the minimum possible fractional decrease in energy?

2. A 50 eV electron is trapped in a finite well. How "far" (in eV) is it from being free if the penetration length of its wave function into the classically forbidden region is 1 nm?

Tutorial on Applications of Schrodinger equation

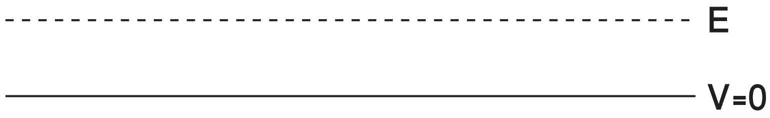
1. Figures (a) through (f) show various kinds of potential steps and obstacles to an electron injected from the left, with energy E. $V(x)$ is shown by solid lines and E by dashed lines. Two or three regions (I, II and III) are also identified. In each case, discuss the following.

   (i) Fields (wavefunctions) in each region—their mathematical form and sketches of their real parts.

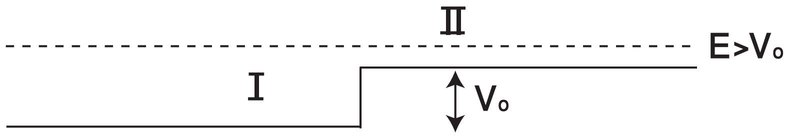
   (ii) Identify the discontinuities from where reflection of the single electron can take place.

   The figures are shown overleaf.

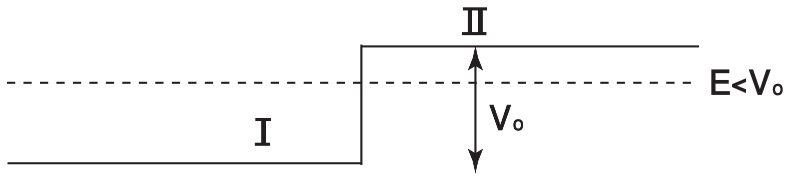
(a)


E
V=0

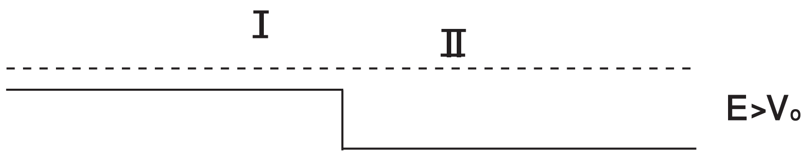
(b)


II
E>Vo
I
Vo

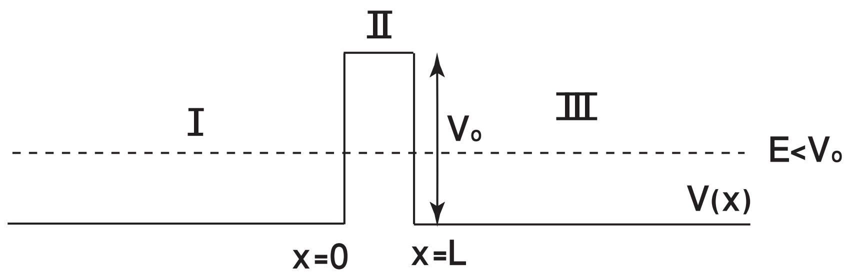
(c)


II
E<Vo
I
Vo

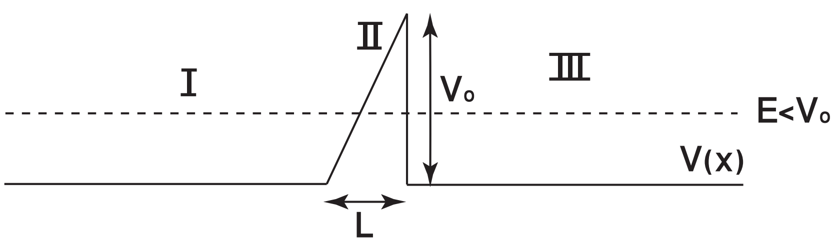
(d)


I
II
E>Vo

(e)


II
I
Vo
III
E<Vo
V(x)
x=0
x=L

(f)


II
I
Vo
III
E<Vo
V(x)
L

Recitation and individual homework 4
Quantum Leakage

In the recitation we will provide outlines to the solution, while you will complete the homework working alone. You will be graded on a coarse scale, with 0, 5, 10 or 15 marks. Solution will be provided after the deadline, Monday 6 May, 10 am. I find it important you do this assignment on your own to obtain a good working knowledge of Schrodinger mechanics.

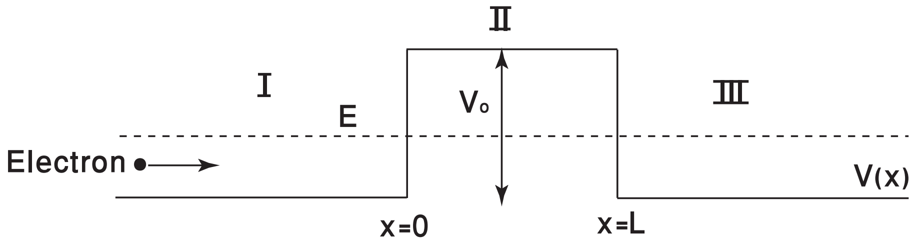


Fig. (a)

Consider the potential energy barrier of length L and height V_0 as shown above. An electron is injected from the left. It has energy $E < V_0$.

(a) Write down the wavefunctions in regions I, II and III. These wavefunctions should include physically plausible terms. The Schrodinger equation (space part) is,

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

(b) Write down the boundary conditions at $x = 0$ and $x = L$.

(c) If a single electron is injected, will it be reflected from the wall at $x = 0$? Can it penetrate through the obstacle and be found at $x > L$?

(d) Can the electron be "really"—I mean physically be found inside the region II? Use the uncertainty principle to answer this question.

(e) Find the probability T that the incident electron from the far left is transmitted into region III.

(f) Now consider the Fig.(b) with, $E < V_0$, $E > W_0$, and $V_0 > W_0$.

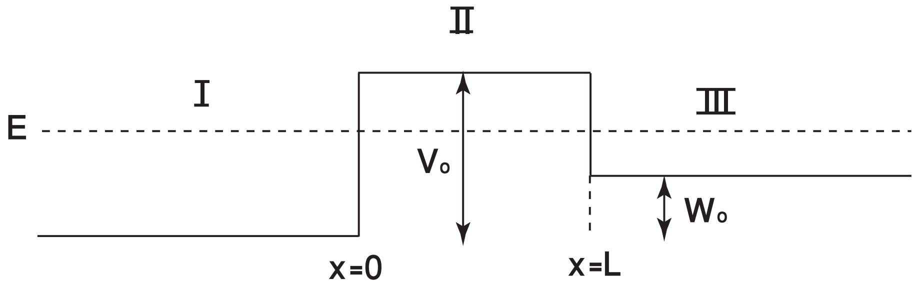


Fig. (b)

Using your result for part (e), find the transmission probability into region III.

(g) If the barrier in figure (a) is to act like a 50:50 beamsplitter, what are the required conditions on E, V_0 and L?

Recitation on aspects of uncertainty principle

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.

1. **(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 it 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.

   <u>**Answer 1:**</u>

   (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,

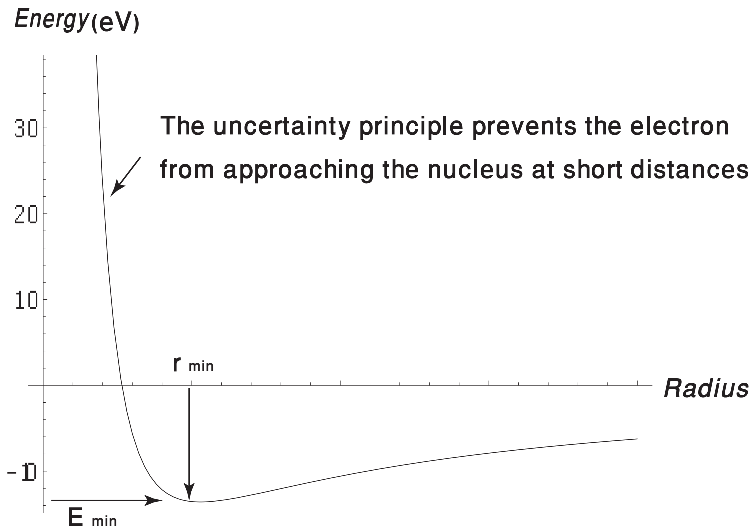
$$\begin{aligned}\text{Total Energy} &= E = K.E + P.E \\ &= \frac{\hbar^2}{2mr^2} - \frac{Ze^2}{4\pi\epsilon_o r}.\end{aligned}$$

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

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

Setting this equal to zero,

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



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.

2. 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: $P = -dE/dV$, 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!

Answer 2:

(a) Using the information provided in Question 1: $\Delta p \sim p$ 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,

$$\begin{aligned} \text{Total Energy} &= E = K.E + P.E \\ &= \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\epsilon_o r}. \end{aligned} \tag{1}$$

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

$$\begin{aligned} \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\epsilon_o r} &= 0 \\ \frac{\hbar^2}{2mr^2} &= \frac{4\pi\epsilon_o r}{e^2} \\ r_{ion} &= \frac{2\pi\epsilon_o \hbar^2}{me^2} = 0.24\,\text{Å}. \end{aligned}$$

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,

$$\begin{aligned} P &= -\frac{dE}{dV} \\ &= -\frac{dE}{dr}\,\frac{dr}{dV} \qquad \text{using the chain rule.} \end{aligned}$$

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),

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

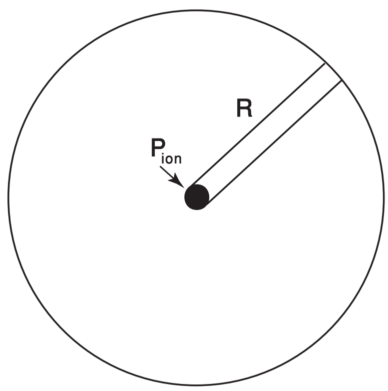
We now substitute the value of the radius, $r = r_{ion}$,

$$\left.\frac{dE}{dr}\right|_{r=r_{ion}} = \frac{-\hbar^2}{m}\left(\frac{1}{r_{ion}}\right)^3 + \frac{e^2}{4\pi\epsilon_o}\left(\frac{1}{r_{ion}}\right)^2 = -3.9\times 10^7\,\mathrm{J\,m^{-1}},$$

resulting in the ionizing pressure,

$$\begin{aligned} P_{ion} &= -\frac{dE}{dr}\,\frac{1}{4\pi r_{ion}^2} \\ &= 5.2\times 10^{13}\ \mathrm{Pa}. \end{aligned}$$

(c)



We assume a spherical planet of radius R and mass M. We determine the 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. An estimate of the density is the proton mass divided by the volume of the atom,

$$\rho = \frac{m_p}{\frac{4}{3}\pi r_{ion}^3} = 2.8 \times 10^4 \text{ kg m}^{-3}. \tag{2}$$

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,

$$\begin{aligned} P_{ion} &= \rho\, g\, R = \frac{\rho\, G\, M}{R} && (3) \\ \Rightarrow R &= \frac{\rho G M}{P_{ion}} = 3.5 \times 10^{-20}\, M \text{ m}. && (4) \end{aligned}$$

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

$$\begin{aligned} \rho = 2.8 \times 10^4 \text{ kg m}^{-3} &= \frac{M}{\frac{4}{3}\pi R^3} && (5) \\ \Rightarrow M &= \frac{4}{3}\, \pi \rho R^3. && (6) \end{aligned}$$

Inserting the value of M into (4) and then back substituting results in,

$$\begin{aligned} M &= 4 \times 10^{26}\, \text{kg}, \\ R &= 1.6 \times 10^7\, \text{m}. \end{aligned}$$

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

Tutorial on relevance of quantum concepts to the classical world

1. A visual inspection of an ant (mass: 0.5 mg) verifies that it is within an uncertainty of 0.7 μm of a given point, apparently stationary. How fast might the ant actually be moving?

2. The uncertainty in the position of a cricket ball of mass 0.145 kg is 1 μm. What is the minimum uncertainty in its speed?

3. 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?

4. The position of a neutron in nucleus is known within an uncertainty of $\sim 5 \times 10^{-15}$ m. At what speeds might we expect to find it moving?

Recitation: Thanks Mr. Planck that your constant is small! Solution

1. A stationary 1 mg grain of sand is found to be at a given location within an uncertainty of 550 nm.

   (a) What is the minimum uncertainty in its velocity?

   (b) Were it moving at this speed, how long would it take to travel 1 μm?

   (c) Can classical mechanics be applied reliably?

   (d) What is a reasonable wavelength of the grain of sand and will it behave as a wave or as a particle?

   (e) What is the minimum uncertainty in its velocity if $h = 6.67 \times 10^{-10}$Js instead of 6.67×10^{-34}Js.

   Answer 1: We are given that,

$$\begin{aligned}\text{Mass of grain} &= m = 1 \text{ mg} = 10^{-6} \text{ kg}\\ \text{Uncertainty in position} &= \Delta x = 550 \text{ nm} = 550 \times 10^{-9} \text{ m.}\end{aligned}$$

   (a) Uncertainty in velocity can be calculated by calculating uncertainty in its momentum. According to uncertainty principle, the minimum uncertainty is approximately,

$$\begin{aligned}\Delta x \ \Delta p &\geq \frac{\hbar}{2}\\ \Rightarrow \Delta p &\geq \frac{\hbar}{2\Delta x} = \frac{1.05 \times 10^{-34}}{2 \times 550 \times 10^{-9} \text{ m}}\\ &= 9.65 \times 10^{-29} \text{ kgms}^{-1}.\end{aligned}$$

   Δp is small because $\hbar$ is small. Now the uncertainty in speed is calculated as,

$$\begin{aligned}\Delta p &= m\Delta v\\ \Delta v &= \frac{\Delta p}{m}\\ &= \frac{9.7 \times 10^{-29} \text{ kg m s}^{-1}}{10^{-6} \text{ kg}}\\ &= 9.65 \times 10^{-23} \text{ m s}^{-1}.\end{aligned}$$

For macroscopic particle $\Delta v \geq \hbar/2(\Delta x)m$ is small because of the very small $\hbar/m$ ratio. Δv becomes significant only if $\hbar$ were large or the mass m decreases. Small $\hbar$ and large m makes the macroscopic classic world "undisturbed" by quantum uncertainties!

(b)

$$\Delta t \approx \frac{1\ \mu\text{m}}{\Delta v} = \frac{10^{-6}}{9.65 \times 10^{-23}}\text{s} = 0.1 \times 10^{17}\ \text{s} \approx 3 \text{ billion years!}$$

The uncertainty in velocity is really really small! An observer would require 3 billion years to notice the grain of sand, supposedly at rest, at a position 1 μm away from its original position. The current age of the solar system is approximately 5 billion years.

(c) Yes uncertainties are extremely small. No device has ever been built, and may never be built that can measure these small velocities. We can safely apply classical mechanics to a grain of sand; there is effectively no uncertainty in position or in momentum. Furthermore, a precision as fine as 10^{-22} m/s is never required in classical mechanics.

(d)

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

Now what momentum should I choose? The uncertainty principle dictates a $\Delta p \sim 9.7 \times 10^{-29}$ kg m s^{-1}. The momentum could therefore have any value between, approximately $-\Delta p/2$ and $\Delta p/2$. Let's choose an extreme value, $p \sim \Delta p/2 \sim 5 \times 10^{-29}$ kg m s^{-1}. Therefore,

$$\lambda \sim \frac{6.67 \times 10^{-34}}{5 \times 10^{-29}} \sim 1.3 \times 10^{-5} \text{ m}.$$

This is such a small wavelength compared to apparatus we might use for macroscopic objects, that for all practical purposes, the grain of sand acts like a particle!

(e) Δv would be $9.65 \times 10 \approx 96$ m/s, if h were this large. This is a huge uncertainty. We are "saved" by the exceedingly small value of h

2. An electron is held in orbit about a proton by electrostatic attraction.

(a) Assume that an "orbiting electron wave" has the same energy an orbiting particle would have if at radius r and of momentum mv. Write an expression for this energy.

(b) If the electron behaves as a classical particle, it must obey $F = ma$. Assuming circular orbit, apply $F = ma$ to eliminate v in favor of r in the energy expression.

(c) Suppose instead that the electron is an orbiting wave, and that the product of the uncertainties in radius r and momentum p is governed by an uncertainty relation of the form $\Delta p \Delta r \approx \hbar$. Also assume that a typical radius of this orbiting wave is roughly equal to the uncertainty Δr, and that a typical magnitude of the momentum is roughly equal to the uncertainty Δp, so that the uncertainty relation becomes $pr \approx \hbar$. Use this to eliminate v in favor of r in the energy expression.

(d) Sketch on the same graph the expressions from parts (b) and (c).

(e) Find the minimum possible energy for the orbiting electron wave, and the value of r to which it corresponds.

Answer 2:

(a) Total energy of an orbiting particle in terms of its kinetic energy and electrostatic potential energy is give by,

$$\begin{aligned} E_{\text{total}} &= \text{K.E.} + \text{P.E.} \\ E_{\text{total}} &= \frac{1}{2}mv^2 + \left[-\frac{ke^2}{r}\right] \\ E_{\text{total}} &= \frac{1}{2}mv^2 - \frac{ke^2}{r}, \end{aligned}$$

where $k = 1/4\pi\epsilon_0$. Therefore total energy of the particle will become,

$$E_{\text{total}} = \frac{1}{2}mv^2 - \frac{e^2}{4\pi\epsilon_0 r}.$$

Hence the energy of "orbiting electron wave" is also,

$$E = \frac{1}{2}mv^2 - \frac{e^2}{4\pi\epsilon_0 r}. \tag{1}$$

(b) Since electron is orbiting in a circular orbit, its centripetal acceleration in its orbit is (v^2/r), while electrostatic force on the electron is (ke^2/r^2), thus,

$$\begin{aligned} F &= ma \\ \frac{ke^2}{r^2} &= m\left(\frac{v^2}{r}\right) \\ \Rightarrow v^2 &= \frac{ke^2}{mr} \\ v^2 &= \frac{e^2}{4\pi\epsilon_0 mr}. \end{aligned}$$

Use this value of v^2 in equation (1),

$$\begin{aligned} E_{\text{classical particle}} &= \frac{1}{2}m\left(\frac{e^2}{4\pi\epsilon_0 mr}\right) - \frac{e^2}{4\pi\epsilon_0 r} \\ &= \frac{1}{2}\left(\frac{e^2}{4\pi\epsilon_0 r}\right) - \frac{e^2}{4\pi\epsilon_0 r} \\ &= \frac{e^2}{8\pi\epsilon_0 r} - \frac{e^2}{4\pi\epsilon_0 r} \\ &= -\frac{e^2}{8\pi\epsilon_0 r}. \end{aligned}$$

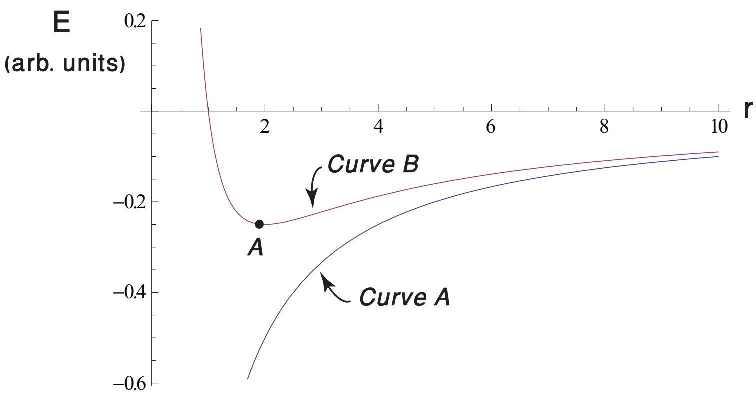
The negative electrostatic potential energy is always of greater magnitude than the positive kinetic energy, so the total energy strictly decreases as r decreases. Hence there is no minimum energy. In the accompanying figure, course A corresponds to the energy of the classical particle, whose energy decreases as r.

(c) Now assuming $pr = \hbar$, we have $p = \hbar/r$ or $v = \hbar/mr$. Therefor equation (1) becomes,

$$\begin{aligned} E_{\text{matter wave}} &= \frac{1}{2}m\left(\frac{\hbar}{mr}\right)^2 - \frac{e^2}{4\pi\epsilon_0 r} \\ &= \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\epsilon_0 r}. \end{aligned}$$

In this case as r decreases, and the wave become more compact, the likely speed increases. The kinetic energy increases faster than the potential decreases, and the total energy at some point must increase. Hence applying uncertainty principle there is a turning point A in the curve labelled B.

(d) The two plots are shown in the figure.



While the energy of a classical particle would monotonically decrease as r decreases, the energy of the matter wave reaches a minimum, and then increases.

(e) The minimum possible energy for the orbiting electron wave can be calculated by setting the derivative of energy with respect to r, to zero.

$$\begin{aligned} E_{\text{matter wave}} &= \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\epsilon_0 r} \\ \frac{dE_{\text{matter wave}}}{dr} &= -\frac{\hbar^2}{mr^3} + \frac{e^2}{4\pi\epsilon_0 r^2} = 0 \\ \Rightarrow\ r &= \frac{4\pi\epsilon_0\hbar^2}{me^2} \\ &= \frac{9\times 10^9\ \text{Nm}^2/\text{C}^2 \times (1.055\times 10^{-34}\ \text{Js})^2}{9.11\times 10^{-31}\times(1.6\times 10^{-19}\ \text{C})^2} \\ &= 5.3\times 10^{-11}\ \text{m}. \end{aligned}$$

This turns out to be astoundingly close to the Bohr radius calculated earlier in class. Inserting this value of r and other constants will give energy for matter wave as follows.

$$E_{\text{matter wave}} = -13.6\ \text{eV}.$$

The energy happens to equal the correct, experimentally determined value, and the radius is indeed the most probable radius at which the electron would be found. That these agree *so closely* is an accident; many approximations have been made. Nevertheless, the uncertainty principle does impose a lower limit on the energy, and it is no accident that the value we obtained is of the correct order of magnitude.

Recitation on infinite well
Solution

1. An electron is confined in an infinite well of 30 cm width.

   (a) What is the ground-state energy?

   (b) In this state, what is the probability that the electron would be found within 10 cm of the left-hand wall?

   (c) If the electron instead has an energy of 1.0 eV, what is the probability that it would be found within 10 cm of the left-hand wall?

   (d) For the 1-eV electron, what is the distance between nodes and the minimum possible fractional decrease in energy?

   <u>Answer 1:</u>

   (a) For an infinite square well, the energy is,

$$E_n = \frac{\pi^2 \hbar^2 n^2}{2mL^2}.$$

   For the ground state, $n = 1$ and the corresponding energy is,

$$\begin{aligned} E_1 &= \frac{\pi^2 \hbar^2}{2mL^2} \\ &= \frac{\pi^2 (1.054 \times 10^{-34}\,\text{J sec})^2}{2(9.1 \times 10^{-31}\,\text{kg})(0.3\,\text{m})^2} \\ &= 6.71 \times 10^{-37}\,\text{J}. \end{aligned}$$

   (b) The wavefunction for an infinite square well is,

$$\begin{aligned} \psi_n &= \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \\ \psi_1 &= \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right). \end{aligned}$$

The probability of finding the electron within 10 cm of the left-hand wall is,

$$\begin{aligned}
P(0 < x < 0.1\,\mathrm{m}) &= \int_0^{0.1} \psi^*(x)\psi(x)dx \\
&= \int_0^{0.1} |\psi(x)|^2 dx \\
&= \frac{2}{L}\int_0^{0.1} \sin^2(\pi x/L)dx \\
&= \frac{2}{L}\int_0^{0.1} \frac{(1-\cos(2\pi x/L))}{2}dx \\
&= \frac{1}{L}\int_0^{0.1} (1-\cos(2\pi x/L))dx \\
&= \frac{1}{L}\left[1 - \frac{\sin(2\pi x/L)}{2\pi/L}\right]_0^{0.1} \\
&= 0.21.
\end{aligned}$$

(c) If the electron has 1.0 eV of energy, then,

$$\begin{aligned}
\frac{\pi^2\hbar^2 n^2}{2mL^2} &= 1.6 \times 10^{-19}\,\mathrm{J} \\
n^2 &= \frac{2mL^2(1.6 \times 10^{-19}\,\mathrm{J})}{\pi^2\hbar^2} \\
&= \frac{2(9.11 \times 10^{-31}\,\mathrm{kg})(0.3\,\mathrm{m})^2(1.6 \times 10^{-19}\,\mathrm{J})}{\pi^2(1.054 \times 10^{-34}\,\mathrm{J\ sec})^2} \\
&= 2.38 \times 10^{17} \\
n &= 4.88 \times 10^{8}.
\end{aligned}$$

With this energy of electron, the probability of finding it within 10 cm of left-hand wall is,

$$\begin{aligned}
P(0 < x < 0.1\,\mathrm{m}) &= \int_0^{0.1} \psi^*(x)\psi(x)dx \\
&= \frac{2}{L}\int_0^{0.1} \sin^2(n\pi x/L)dx \\
&= \frac{2}{L}\int_0^{0.1} \frac{(1-\cos(2n\pi x/L))}{2}dx \\
&= \frac{1}{L}\int_0^{0.1} (1-\cos(2n\pi x/L))dx \\
&= \frac{1}{L}\left[1 - \frac{\sin(2n\pi x/L)}{2n\pi/L}\right]_0^{0.1} \\
&= 0.33.
\end{aligned}$$

(d) We know that,

$$\begin{aligned} L &= n\frac{\lambda}{2} \\ \lambda &= \frac{2L}{n}. \end{aligned}$$

Now the distance between the nodes is,

$$\begin{aligned} \frac{\lambda}{2} &= \frac{L}{2} = \frac{0.3}{4.8 \times 10^8} \\ &= 6.15\,\mathring{A}. \end{aligned}$$

The maximum possible fractional decrease in energy is thus,

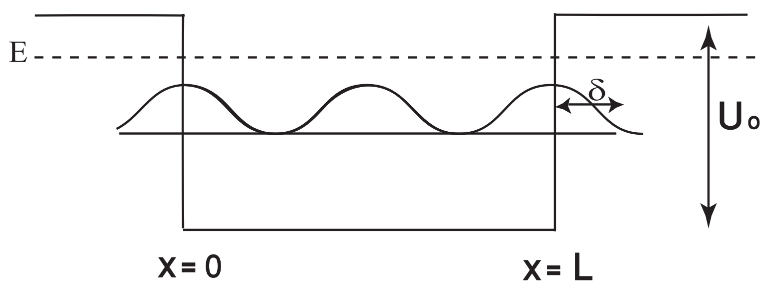
$$\begin{aligned} \frac{\Delta E}{E} &= \frac{E_n - E_{n-1}}{E_n} \\ &= \frac{n^2 - (n-1)^2}{n^2} \\ &= \frac{2}{n} - \frac{1}{n^2}, \end{aligned}$$

since $n = 4.8 \times 10^8$, the minimum fractional decrease in energy is,

$$\frac{\Delta E}{E} = 4.1 \times 10^{-9}\,\mathrm{J}.$$

2. A 50 eV electron is trapped in a finite well. How "far" (in eV) is it from being free if the penetration length of its wave function into the classically forbidden region is 1 nm?

Answer 2:

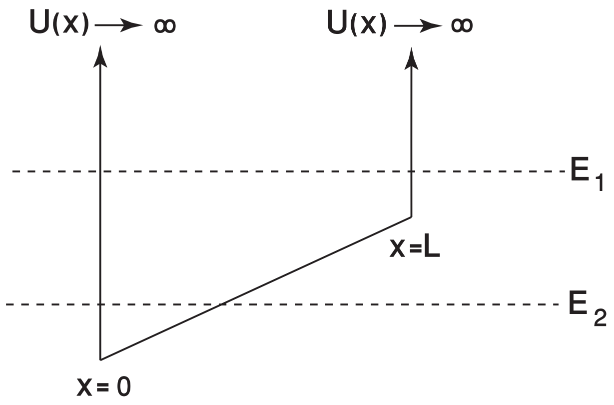


The penetration depth δ is given by,

$$\begin{aligned}
\delta &= \frac{\hbar}{\sqrt{2m(U_0 - E)}} = 1 \times 10^{-9}\,\mathrm{m} \\
2m(U_0 - E) &= \frac{\hbar^2}{(1 \times 10^{-9}\,\mathrm{m})^2} \\
U_0 - E &= \frac{\hbar^2}{2m(1 \times 10^{-9}\,\mathrm{m})^2} \\
&= 38.2\,\mathrm{meV}.
\end{aligned}$$

Tutorial on infinite well

1. Consider a particle that is bound inside an infinite well whose "floor" is sloping as shown on the next page.



Sketch a plausible wave function when the energy is E_1 and when the energy is E_2.

2. In an infinite well, consider the 1st excited state, i.e., $n = 2$.

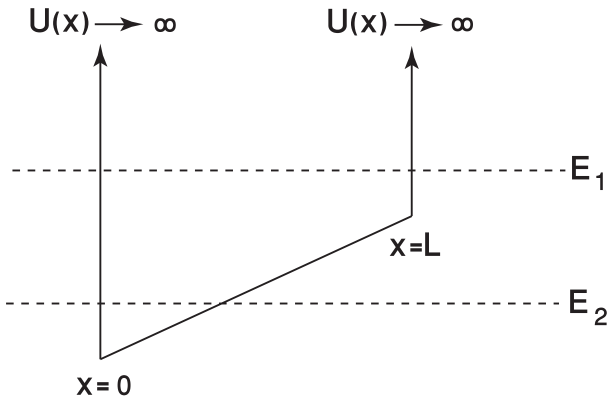
(a) What is the most probable position of the particle after a measurement has been made?

(b) What is the average position, $\langle x \rangle$?

3. The nuclear potential that binds protons and neutrons in the nucleus of an atom is often approximated by a square well. Imagine a proton confined in an infinite square well of length 10^{-5} nm, a typical nuclear diameter. Calculate the wavelength and energy associated with the photon that is emitted when the proton undergoes a transition from the first excited state ($n = 2$) to the ground state ($n = 1$). In what region of the electromagnetic spectrum does this wavelength belong?

Tutorial on infinite well
Solution

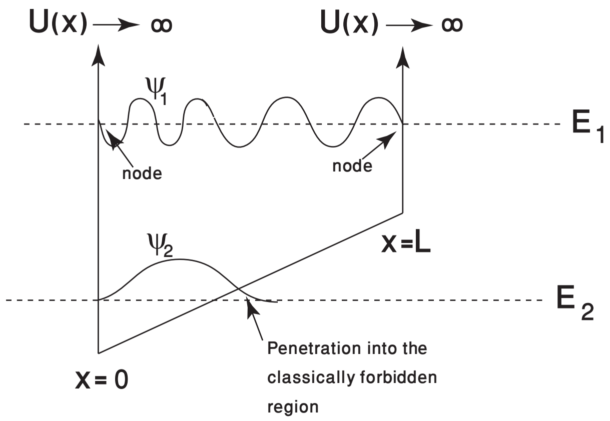
1. Consider a particle that is bound inside an infinite well whose "floor" is sloping as shown on the next page.



Sketch a plausible wave function when the energy is E_1 and when the energy is E_2.

Answer 1:

The plausible wavefunctions are shown in the Figure.



The wavefunction $\psi_1(x)$ corresponds to energy E_1 and $\psi_2(x)$ corresponds to energy E_2. If $E > U(x)$, the wavefunction is $\propto \exp\left(\frac{i\sqrt{2m(E-U(x))}}{\hbar}\right)$, which is oscillatory. Larger the value of $E - U(x)$, higher the value of $k = \sqrt{\frac{2m(E-U(x))}{\hbar}}$ and shorter the wavelength. If $E < U(x)$, the wavefunction decays (damps). Note that the wavelength for $\psi_1(x)$ is not uniform, rather the wavelength increases, k decreases as $E - U(x)$ decreases in going from left to right.

2. In an infinite well, consider the 1st excited state, i.e., $n = 2$.

(a) What is the most probable position of the particle after a measurement has been made?

(b) What is the average position, $\langle x \rangle$?

Answer 2:

The wavefunction for an infinite well is,

$$\begin{aligned} \psi_n(x) &= \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \\ \text{For first excited state, } n = 2, & \\ \psi_2(x) &= \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right) \\ \text{and the probability is,} & \\ P_2(x) &= |\psi_2(x)^* \psi_2(x)| \\ &= \frac{2}{L} \sin^2\left(\frac{2\pi x}{L}\right). \end{aligned}$$

To find the most probable position, we have to maximize $P_2(x)$.

$$\begin{aligned} \frac{dP_2(x)}{dx} &= 2\left(\frac{2}{L}\right) \sin\left(\frac{2\pi x}{L}\right) \cos\left(\frac{2\pi x}{L}\right) \left(\frac{2\pi}{L}\right) \\ &= 2\pi\left(\frac{4}{L^2}\right) \sin\left(\frac{2\pi x}{L}\right) \cos\left(\frac{2\pi x}{L}\right) \end{aligned}$$

The quantity $\frac{dP_2(x)}{dx} = 0$ when $x = 0,\ L/4,\ L/2,\ 3L/4,\ L$ but when $x = 0,\ L/2,\ L,$ the wavefunction $\psi_2(x) = 0$.

Thus at $x = 0,\ L/2,\ L$, the probability of finding the particle is zero. The most probable positions are $x = L/4$, and $x = 3L/4$.

(b) The average position is given by the following,

$$
\begin{aligned}
\langle x \rangle &= \int_0^L x\,\psi_2^*(x)\psi_2(x)dx \\
&= \int_0^L x\,|\psi_2(x)|^2\,dx \\
&= \frac{2}{L}\int_0^L x\,\sin^2(2\pi x/L)dx \\
&= \frac{2}{2L}\int_0^L x\,(1-\cos(4\pi x/L))dx \\
&= \frac{1}{L}\int_0^L xdx - \frac{1}{L}\int_0^L x\cos(4\pi x/L)dx \\
&= \frac{L}{2} - 0 \\
&= \frac{L}{2}.
\end{aligned}
$$

3. The nuclear potential that binds protons and neutrons in the nucleus of an atom is often approximated by a square well. Imagine a proton confined in an infinite square well of length 10^{-5} nm, a typical nuclear diameter. Calculate the wavelength and energy associated with the photon that is emitted when the proton undergoes a transition from the first excited state ($n = 2$) to the ground state ($n = 1$). In what region of the electromagnetic spectrum does this wavelength belong?

Answer 3:

In a square well, the energy that corresponds to n'th energy level is,

$$E_n = \frac{\pi^2\hbar^2 n^2}{2mL^2}.$$

When a proton undergoes a transition from the first excited state ($n = 2$) to the ground state ($n = 1$), the energy of emitted photon is,

$$
\begin{aligned}
\Delta E_{2\to 1} &= \frac{\pi^2\hbar^2}{2mL^2}(2^2 - 1^2) \\
&= \frac{3\pi^2\hbar^2}{2mL^2} \\
&= \frac{3\pi^2(1.054\times 10^{-34}\,\mathrm{Js})^2}{2(1.67\times 10^{-27}\,\mathrm{kg})(10^{-14}\,\mathrm{m})^2} \\
&= 9.8\times 10^{-15}\,\mathrm{J}.
\end{aligned}
$$

The wavelength of emitted photon is,

$$\begin{aligned}
\lambda &= \frac{hc}{\Delta E} \\
&= \frac{(6.63 \times 10^{-34}\,\mathrm{Js})(3 \times 10^{8}\,\mathrm{m/s})}{9.8 \times 10^{-15}\,\mathrm{J}} \\
&= 2 \times 10^{-11}\,\mathrm{m}.
\end{aligned}$$