A

Homework: QM3

A particle trapped in $0 < x < L$ in a 1 dimensional infinite potential well has energy levels $E_n = n^2\hbar^2\pi^2/(2mL^2)$. (a) Find the width of the box if the ground state energy equals 13.6eV (the absolute value of the binding energy of the hydrogen atom). (b) Find the width of the box if a transition from the n=2 to n=1 state emits a photon with l=122nm (as in hydrogen). What is the ground state energy of this box? (c) Describe the differences between the 1 dimensional infinite potential and that of a real hydrogen atom which might account for the differences between your answers for (a) and (b)

The energy levels in an infinite well are given analytically as

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}, \tag{A.1}$$

where n is the *principal quantum number* (one of four numbers used to describe the state of an electron—you'll meet the rest in stage 2), m is the mass of the particle and L is the width of the box.

[*The question does not state which particle it is being trapped, so assume it is an electron from the context of the problem (the binding energy of an electron in a hydrogen atom). Normally this will be given in an exam to avoid confusion.*]

In (a), we are interested in the width of the box. Rearranging gives

$$L^2 = \frac{n^2\pi^2\hbar^2}{2E_n m}. \tag{A.2}$$

The bound state energies in a hydrogen atom are

$$E_n = \frac{E_1}{n^2} = \frac{-13.6\,\text{eV}}{n^2}, \tag{A.3}$$

for $n \in \mathbb{Z}$. [*n strictly takes on only positive values, and $n = 1$ is, again, the ground state.*] These are the eigenenergies of the time-independent Schrödinger equation. Here, we consider the absolute value of this (basically, just readjusting where we take our reference energy $E = 0$).

In an infinite well, the ground state is the $n = 1$ state (there is no state with $n = 0$, which corresponds to zero wave function).

Equating the ground state ($n = 1$) energy (in joules) of the electron in a hydrogen atom with the with the ground state of an infinite well, one finds that

$$\begin{aligned} L^2 &= \frac{1^2 \times \pi^2\hbar^2}{2 \times -13.6 \times 1.60 \times 10^{-19} \times 9.11 \times 10^{-19}} \\ \implies L &= 1.66 \times 10^{-10}\,\text{m}. \end{aligned} \tag{A.4}$$

For (b), we wish to find the energy difference between the $n = 2$ (first excited state) and $n = 1$ (ground state), as this energy is the energy of the photon emitted. Thus,

$$E_2 - E_1 = \frac{2^2\pi^2\hbar^2}{2mL^2} - \frac{1^2\pi^2\hbar^2}{2mL^2} = \frac{3 \times \pi^2\hbar^2}{2mL^2}. \tag{A.5}$$

We are given that the wavelength of the emitted photon is $\lambda = 122$ nm, so the photon energy is given by

$$E_\gamma = \frac{hc}{\lambda} \tag{A.6}$$

Equating $E_2 - E_1 = E_\gamma$ gives

$$\frac{3\pi^2\hbar^2}{2mL^2} = \frac{hc}{\lambda}, \tag{A.7}$$

so this implies that

$$L^2 = \frac{3\pi^2\hbar^2\lambda}{2mhc} = \frac{3\pi^2\hbar^2(122\times10^{-9})}{2\times9.11\times10^{-31}hc} \implies L = 3.33\times10^{-10}\text{ m}. \tag{A.8}$$

For (c), the hydrogen atom has a 3D spherical structure, while the infinite potential well is a 1D model. The hydrogen atom has a Coulomb potential that depends on $1/r$, whereas the infinite potential well has a constant potential (infinite) outside the well and zero inside. [*You will study the mathematics of the hydrogen atom in stage 2 and 3 quantum mechanics—it is actually a very advanced topic!*]

An electron is trapped in a 1 dimensional finite well, where $U = 0$ for $0 < x < L$ and $U = 6E_{1\infty}$ for $x < 0$ and $x > L$ where $E_{1\infty} = \hbar^2\pi 2/(2mL^2)$, i.e. the ground state energy of an infinite well of the same width. This finite well potential has 3 bound states, with $E_1 = 0.625E_{1\infty}$, $E_2 = 2.43E_{1\infty}$, $E_3 = 5.09E_{1\infty}$, and $L = 1$ nm. (a) What is the maximum wavelength which will eject an electron from the ground state? (b) What is the kinetic energy of an electron which is ejected from the first excited state by a photon of wavelength $\lambda = 500$ nm.

For (a), we need to consider the energy difference between the ground state and the potential energy outside of the well, U_0, in order to calculate the minimum energy required to eject an electron from the ground state. The energy difference is $\Delta E = U_0 - E_1$. We associate ΔE with the energy released during this ejection, which is exactly the energy of the photon hc/λ. So,

$$\frac{hc}{\lambda} = U_0 - E_1 = (6-0.625)E_{1\infty} = 5.375\frac{\hbar^2\pi^2}{2mL^2}. \tag{A.9}$$

Rearranging, we find

$$\begin{aligned}\lambda &= \frac{2hcL^2m}{5.375\hbar^2\pi^2}\\ &= \frac{2\times 6.63\times 10^{-34}\times 3.3.00\times 10^{8}\times(1.00\times 10^{-9})^2\times 9.11\times 10^{-31})}{5.375\times(1.05\times 10^{-34})^2\pi^2}\\ \implies \lambda &= 614\,\text{nm}.\end{aligned} \tag{A.10}$$

To 1 s.f., $\lambda = 600$ nm.

In (b), we are interested in the kinetic energy of an electron ejected from its first excited state (the $n = 2$ state—remember that in infinite and finite wells we start counting at $n = 1$).

The photon energy is

$$E = \frac{hc}{\lambda} = \frac{6.63\times 10^{-34}\times 3.00\times 10^{8}}{500\times 10^{-9}} = 3.98\times 10^{-19}\,\text{J} \tag{A.11}$$

[*NB: We would never quote an energy of this order of magnitude in joules. When quoting the answer, we would need to convert to eV. However, we need to use this in subsequent calculations, so we will keep it in J.*]

The ejection energy is then $\Delta E = U_0 - E_2 = (6 - 2.43)E_{1\infty} = \cdots = 2.15\times 10^{-19}$ J which is calculated in the same way as (a).

Now, we can find the kinetic energy, T, by subtracting the energy of the first excited state ($E_2 = 2.43E_{1\infty}$) from the photon's energy:

$T = E_\gamma - E_2 = 3.98\times 10^{-19}\text{J} - 2.15\times 10^{-19}\text{ J} = 1.84\times 10^{-19}$ J.

To 1 s.f., $T = 1$ eV.

A wave function which is a solution of the time-dependent Schrödinger equation (and not the time-*in*dependent Schrödinger equation) is given

by $\Psi(t=0,x) = A\psi_1(x) + B\psi_2(x)$, where ψ_1 and ψ_2 are different solutions of the time-independent Schrödinger equation (e.g., for a particle in a 1d infinite well). (a) Write $\Psi(t,x)$ for $t \neq 0$. (b) Determine the probability density and probability of finding a particle within a distance $\mathrm{d}x$ of x at a time t. State whether the probability density and corresponding probability is time-dependent or time-independent

[*I have corrected this question from the problem sheet.*]

The wave function at $t = 0$ is given by a linear superposition of states in e.g., an infinite well. These states have different energies, E_1 and E_2. As the wave function evolves in time, each state picks up a phase factor $\exp(-iE_n t/\hbar)$. Thus, the full (yes, for all time!) evolution of the wave function is

$$\Psi(t,x) = A\psi_1(x)\mathrm{e}^{-iE_1 t/\hbar} + B\psi_2(x)\mathrm{e}^{-iE_2 t/\hbar}, \tag{A.12}$$

where $|A|^2 + |B|^2 = 1$ determine the probabilities of obtaining the individual states ψ_1 and ψ_2 upon measurement of the wave function (i.e., the probability at which the wave function will collapse into a particular state, ψ_1 or ψ_2).

For (b), to find the probability to find the particle within dx of x at time t, we first need to calculate the probability density function. The probability density is given by the square of the absolute value of the wavefunction. For the given wavefunction, we have:

$$\Psi(t,x) = A\psi_1(x)\mathrm{e}^{-iE_1 t/\hbar} + B\psi_2(x)\mathrm{e}^{-iE_2 t/\hbar}. \tag{A.13}$$

Taking the complex conjugate of the wavefunction, we get:

$$\Psi^*(t,x) = A^*\psi_1^*(x)\mathrm{e}^{iE_1 t/\hbar} + B^*\psi_2^*(x)\mathrm{e}^{iE_2 t/\hbar}. \tag{A.14}$$

Now, we can find the probability density function by multiplying the wavefunction and its complex conjugate:

$$|\Psi(t,x)|^2 = \Psi^*(t,x)\Psi(t,x), \tag{A.15}$$

which leads to

$$|\Psi(t,x)|^2 = |A|^2|\psi_1(x)|^2 + |B|^2|\psi_2(x)|^2 \\ + A^*B^*\psi_1^*(x)\psi_2^*(x)\mathrm{e}^{i(E_1-E_2)t/\hbar} + AB\psi_1(x)\psi_2(x)\mathrm{e}^{-i(E_1-E_2)t/\hbar}. \tag{A.16}$$

The probability to find the particle within dx of x at time t is given by:

$$P(x,t)dx = |\Psi(t,x)|^2 dx \tag{A.17}$$

From the above expression for $|\Psi(t,x)|^2$, we can see that it consists of time-independent terms $|A|^2|\psi_1(x)|^2$ and $|B|^2|\psi_2(x)|^2$, and time-dependent terms $A^*B^*\psi_1^*(x)\psi_2^*(x)\mathrm{e}^{i(E_1-E_2)t/\hbar}$ and $AB\psi_1(x)\psi_2(x)\mathrm{e}^{-i(E_1-E_2)t/\hbar}$. Therefore, the probability to find the particle within dx of x at time t is dependent on time.