Part IB — Quantum Mechanics Example Sheet 1

Supervised by Dr Warnick Examples worked through by Christopher Turnbull

Michaelmas 2017

The first electron has wavelength $\lambda_1 = 3 \times 10^{-7}$ m, and moves at the speed of light, so frequency ν_1 is given by

$$\nu_1 = \frac{c}{\lambda_1} = \frac{3.00 \times 10^8}{3 \times 10^{-7}} = 1 \times 10^{15} \text{ s}^{-1}$$

Similarly $\nu_2 = 0.6 \times 10^{15}$. If W is the minimum energy needed to liberate an electron from Potassium then

$$K_1 = h\nu_1 - W$$

$$K_2 = h\nu_2 - W$$

where K_1, K_2 are the maximum kinetic energy of the liberated electrons. Thus the value of h is given by

$$h = \frac{K_1 - K_2}{\nu_1 - \nu_2} = \frac{1.6 \times (1.60 \times 10^{-19})}{0.4 \times 10^{15}} = 6.4 \times 10^{-34}$$

Thus

$$W = h\nu_1 - K_1$$

= $6.4 \times 10^{-19} - 2.1 \times (1.60 \times 10^{-19})$
= $3.04 \times 10^{-19} \text{ J}$
= 1.9 eV

Let the light have energy flux $E=10^{-10}\rm Jm^{-2}s^{-1}$, with the wavelength $\lambda=5\times10^{-7}$. The energy of one photon is given by

$$E_p = \frac{hc}{\lambda}$$
= $\frac{6.63 \times 10^{-34} \times 3 \times 10^8}{5 \times 10^{-7}}$
= $3.987 \times 10^{-19} \text{ J}$

Take human eye to have area 1 cm² = 10^{-4} m², so energy flux E_e entering human eye is $E_e = 10^{-14} \mathrm{Jm}^{-2} \mathrm{s}^{-1}$.

Thus number of photons entering the eye N is given as

$$N = \frac{E_e}{E_p} \approx 2.51 \times 10^5$$

Classical equations of motion imply that the total energy E_n for an electron at level n ($n = 1, 2, \cdots$) for the electron must be constant, and is given by

$$E_n = \frac{1}{2}mv_n^2 - \frac{e^2}{4\pi\varepsilon_0} \frac{1}{r_n}$$

Resolving radial acceleration gives

$$\frac{mv_n^2}{r_n} = \frac{e^2}{4\pi\varepsilon_0} \frac{1}{r_n^2} \quad (1)$$

which simplifies are expression for energy levels to

$$E_n = -\frac{1}{2}mv_n^2$$

Next, angular momentum quantisation yields

$$mv_n r_n = n\hbar$$
 (2)

Rearranging (1) and (2)

$$r_n = \frac{e^2}{4\pi\varepsilon_0} \frac{1}{mv_n^2} \qquad r_n = \frac{n\hbar}{mv_n}$$

Thus setting equal and solving for v_n gives

$$v_n = \frac{1}{n\hbar} \frac{e^2}{4\pi\varepsilon_0} = c\alpha \frac{1}{n}$$

where $\alpha = e^2/4\pi\varepsilon_0\hbar c$ is the fine structure constant. Substituting this into the expression for energy gives

$$E_n = -\frac{1}{2}mc^2\alpha^2 \frac{1}{n^2}$$

- (i) It is consistent. $\alpha \approx \frac{1}{137}$, so the highest speed an electron can have is $\frac{1}{137}c$ (when n=1, this decreases for larger n), which is less that 1% of the speed of light.
- (ii) Suppose th electron makes a transition between levels n' and n, (with n' > n say), accompanied by emission or a photon of frequency ν . Then

$$h\nu = E_{n'} - E_n = \frac{1}{2}mc^2\alpha^2\left(\frac{1}{n^2} - \frac{1}{n'^2}\right)$$

 $E = \frac{hc}{\lambda}$, so smallest wavelength \Rightarrow most amount of energy, which is emitted when the electron falls from 'infinity' to level 1, ie. $(1/n^2 - 1/n'^2) = 1$. ie.

$$\lambda = \frac{hc}{E}$$

$$= \frac{2hc}{mc^2\alpha^2}$$

$$= \frac{4\pi\hbar}{mc\alpha^2}$$

$$= \frac{e^2}{\varepsilon_0 c} \frac{4\pi\varepsilon_0\hbar c}{e^2} \frac{1}{mc\alpha^2}$$

$$= \frac{e^2}{\varepsilon_0 mc^2\alpha}$$

Bohr radius is given by:

$$r_1 = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$$

Bohr radius r_1 and corresponding (n=1) radius r_1' of muon are given by

$$r_1 = \frac{\hbar}{m_e c \alpha} \qquad r_1' = \frac{\hbar}{m_m c \alpha}$$

where m_e is the mass of the electron, and $m_m = 207m_e$ is the mass of the muon

So the radius the n=1 state of muonic Hydrogen is 207 times smaller than normal Hydrogen.

Given $\psi_0(x) = C_0 e^{-x^2/2\alpha}$, we calculate

$$\psi_0'(x) = -\frac{x}{\alpha}\psi_0(x)$$
 and $\psi_0''(x) = -\frac{1}{\alpha}\psi_0(x) + \frac{x^2}{\alpha^2}\psi_0(x)$

Substituting into the time-indep SE gives

$$-\frac{\hbar^2}{2m} \left(-\frac{1}{\alpha} + \frac{x^2}{\alpha^2} \right) \psi_0 + \frac{1}{2} K x^2 \psi_0 = E_0 \psi_0$$

Comparing constants and x^2 coefficients respectively

$$\frac{\hbar^2}{2m\alpha} = E_0$$
 and $\frac{\hbar^2}{2m} \frac{1}{\alpha^2} = \frac{1}{2}K$

Thus $\alpha=\sqrt{\frac{\hbar^2}{Km}}$ and hence energy eigenvalue $E_0=\frac{\hbar}{2}\sqrt{\frac{K}{m}}$. Similarly, given $\psi_1(x)=C_1xe^{-x^2/2\alpha}=x\phi(x)$, where $\phi(x)=C_1e^{-x^2/2\alpha}$,

Similarly, given
$$\psi_1(x) = C_1 x e^{-x^2/2\alpha} = x\phi(x)$$
, where $\phi(x) = C_1 e^{-x^2/2\alpha}$,

$$\psi_1'(x) = \phi(x) - \frac{x^2}{\alpha}\phi(x)$$
 and $\psi_1''(x) = \frac{-x}{\alpha}\phi(x) - \frac{2x}{\alpha}\phi(x) + \frac{x^3}{\alpha^2}\phi(x)$

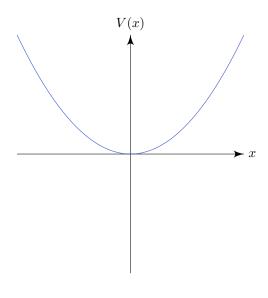
Substituting into time-indep SE yields,

$$-\frac{\hbar^2}{2m}\left(-\frac{3x}{\alpha} + \frac{x^3}{\alpha^2}\right)\phi(x) + \frac{1}{2}Kx^2x\phi(x) = E_1x\phi(x)$$

Comparing x and x^3 coefficients respectively,

$$\frac{3\hbar^2}{2m\alpha} = E_1$$
 and $\frac{\hbar^2}{2m} \frac{1}{\alpha^2} = \frac{1}{2}K$

Hence as before $\alpha = \sqrt{\frac{\hbar^2}{Km}}$ and $E_1 = 3E_0 = \frac{3\hbar}{2}\sqrt{\frac{K}{m}}$



Wavefunction $\Psi(x,t)$ under one-dimensional harmonic oscillator potential $V(x) = \frac{1}{2}Kx^2$ has time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+\frac{1}{2}Kx^2\Psi$$

For separable $\Psi(x,t) = \psi(x)f(t)$, have solutions of type

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$$
 with $H\psi = E\psi$

(i) $\Psi(x,0) = \psi_0(x) \Rightarrow \psi(x) = \psi_0(x)$ and $E = \frac{\hbar}{2} \sqrt{\frac{K}{m}}$ from question 5, so we have

$$\Psi(x,t) = C_0 e^{-x^2/2\alpha} \exp\left(-\frac{i}{2}\sqrt{\frac{K}{m}}t\right)$$

For some normalisation constant C_0

(ii) Similarly $\psi(x) = \psi_1(x)$ and again using results for E from question 5,

$$\Psi(x,t) = C_1 x e^{-x^2/2\alpha} \exp\left(-\frac{3i}{2}\sqrt{\frac{K}{m}}t\right)$$

For some normalisation constant C_1

(iii) For $\Psi(x,0) = \frac{1}{2}(\sqrt{3}\psi_0(x) - i\psi_1(x)) = \psi(x)$, and solving $H\psi = E\psi$ for E, ψ_0 part only has constant and x^2 terms, whereas ψ_1 only contains x and x^3 terms. Thus from parts (i) and (ii) we have

$$E = \frac{1}{2}(\sqrt{3}E_0 - iE_1)$$
$$= \frac{\sqrt{3} - 3i}{2} \left(\frac{\hbar}{2}\sqrt{\frac{K}{m}}\right)$$

Thus

$$\Psi(x,t) = \frac{1}{2}(\sqrt{3}\psi_0(x) - i\psi_1(x)) \exp\left(-\frac{3 - i\sqrt{3}}{4}\sqrt{\frac{K}{m}}t\right)$$

Note that $\Psi(x,t) = C\gamma(t)^{-1/2} \exp(-x^2/2\gamma(t))$ is not separable, V=0. t -dep SE

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+\frac{1}{2}Kx^2\Psi$$

Calculating the partial derivatives

$$\begin{split} \frac{\partial \Psi}{\partial t} &= -\frac{1}{2} \gamma' C \gamma^{-3/2} \exp(-x^2/2\gamma) + C \gamma^{-1/2} \left(\frac{x^2}{2\gamma^2} \gamma' \exp(-x^2/2\gamma) \right) \\ &= \left(-\frac{1}{2} \frac{\gamma'}{\gamma} + \gamma' \frac{x^2}{2\gamma^2} \right) C \gamma^{-1/2} \exp(-x^2/2\gamma) \\ &= \left(-\frac{1}{2} \frac{\gamma'}{\gamma} + \gamma' \frac{x^2}{2\gamma^2} \right) \Psi \end{split}$$

and

$$\begin{split} \frac{\partial^2 \Psi}{\partial x^2} &= \frac{\partial}{\partial x} \left[-\frac{x}{\gamma} \Psi \right] \\ &= -\frac{1}{\gamma} \Psi + \frac{x^2}{\gamma^2} \Psi \end{split}$$

So t-dep SE becomes

$$i\hbar\left(-\frac{1}{2}\frac{\gamma'}{\gamma}+\gamma'\frac{x^2}{2\gamma^2}\right)\Psi=-\frac{\hbar^2}{2m}\left(-\frac{1}{\gamma}+\frac{x^2}{\gamma^2}\right)\Psi$$

Comparing constant and x^2 coefficients repectively,

$$-i\hbar \frac{1}{2} \frac{\gamma'}{\gamma} = \frac{\hbar^2}{2m} \frac{1}{\gamma}$$
 and $i\hbar \frac{\gamma'}{2\gamma^2} = -\frac{\hbar^2}{2m} \frac{1}{\gamma^2}$

Both reveal that

$$\gamma' = \frac{i\hbar}{m}$$
 and hence $\gamma = \alpha + \frac{i\hbar}{m}t$

where $\alpha = \gamma(0)$

Probability density given as

$$|\Psi(x,t)|^2 = \frac{|C|^2}{|\gamma(t)|} e^{-\alpha x^2/|\gamma(t)|^2}$$

localised around x = 0 on scale

$$\frac{|\gamma(t)|}{\sqrt{\alpha}}$$
 solution "diffuses"

```
how quickly does solution "diffuse"? Time scale m\alpha/\hbar
```

For
$$m=m_e$$
, and $\sqrt{\alpha}=10^{-12}$ m \Rightarrow time scale $\sim 10^{-20}$ s
For $m=10^{-6}$ kg, $\sqrt{\alpha}=10^{-6}$ m, \Rightarrow time scale $\sim 10^{16}$ s.

(i)

$$H\psi_1 = E\psi_1$$

$$H\psi_2 = E\psi_2$$

Time indep SE with $V(x) \to 0$ rapidly, is

Time-indep SE is

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

Note that

$$\det \begin{pmatrix} \psi_1 & \psi_2 \\ \psi_1' & \psi_2' \end{pmatrix} = \psi_1 \psi_2' - \psi_2 \psi_1'$$

- (ii)
- (iii)

Time dependent SE is

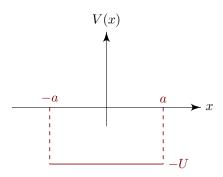
$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+-U\delta(x)\Psi$$

Integrating from $x - \varepsilon$ to $x + \varepsilon$ gives

$$\int_{x-\varepsilon}^{x+\varepsilon} i\hbar \frac{\partial \Psi}{\partial t} \, \mathrm{d}x = -\frac{\hbar^2}{2m} \left[\frac{\partial \Psi}{\partial x} \right]_{x-\varepsilon}^{x+\varepsilon} - U\Psi$$

Taking $\frac{\partial \Psi}{\partial t}$ to be sufficiently smooth, LHS = 0 and we have

$$\left[\frac{\partial\Psi}{\partial x}\right]_{x-\varepsilon}^{x+\varepsilon} = -\frac{2mU}{\hbar^2}\Psi$$



Seek energy functions and eigenvalues given by

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

with energies in range -U < E < 0

SE becomes

$$\underbrace{-\frac{\hbar^2}{2m}\psi'' = (E+U)\psi}_{|x| < a} \text{ and } \underbrace{-\frac{\hbar^2}{2m}\psi'' = E\psi}_{|x| > a}$$

Set

$$U+E=rac{\hbar^2 k^2}{2m}$$
 and $E=rac{-\hbar^2 \kappa^2}{2m}$

$$k > 0$$
 and $\kappa > 0$

then SE is

$$\psi'' + k^2 \psi = 0$$
 and $\psi'' - \kappa^2 \psi = 0$

$$|x| < a$$
 and $|x| > a$

At $x = \pm a$, ψ , ψ' continuous (ψ'' discontinuous, matching step in V(x)) [Integrate SE from $a - \varepsilon$ to $a + \varepsilon$, then provided U, ψ bounded, find $[\psi']_{a-\varepsilon}^{a+\varepsilon} \to 0 \text{ as } \varepsilon \to 0^+]$

Consider *odd parity* solutions, ie. those with $\psi(-x) = -\psi(x)$,

$$\psi = \begin{cases} A \sin kx & \text{if } |x| < a \\ Be^{-\kappa x} & \text{if } x > a \end{cases}$$

Note the solution for x < -a fixed by parity. Matching at x = a,

$$\psi \operatorname{cts} : A \sin ka = Be^{-\kappa a}$$

$$\psi'$$
 cts : $kA\cos ka = -B\kappa e^{-\kappa a}$

These equations give same solution for A or B iff:

$$\kappa \tan ka = -k$$

To find when solutions exists it is convenient to set

 $\xi = ak$, $\eta = a\kappa$ dimensionless and positive

So

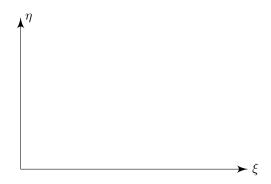
$$\eta = -\frac{\xi}{\tan \xi}$$

but also

$$\xi^2 + \eta^2 = \frac{2ma^2U}{\hbar^2}$$
 from definitions of k and κ

Intersection of $\nu = \xi \tan \xi$ with circle of $(\text{radius})^2 = \frac{2ma^2U}{\hbar^2}$. Have energy eigenstate for each point of intersection $(a, U \text{ fixed parameters, determining } \xi, \nu \text{ determines } E)$

We can look for solutions by plotting these two equations. We first plot the curve $\eta = -\frac{\xi}{\tan \xi}$:



The other equation is the equation of a circle. Depending on the size of the constant $2ma^2U/\hbar^2$, there will be a different number of points of intersections.

Can see that circle must have radius $\geq \frac{\pi}{2}$ for intersection; anything smaller will produce no intersections, ie. no intersections if

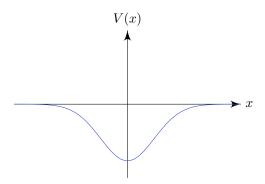
$$2ma^2U/\hbar^2<\left(\frac{\pi}{2}\right)^2$$

which rearranges to

$$aU^2 < (\pi\hbar)^2/8m$$

as required

Potential $V(x) = -\frac{\hbar^2}{2m} \operatorname{sech}^2 x$



Time-indep SE is

$$-\frac{\hbar^2}{2m}\psi''(x) - \frac{\hbar^2}{m}\operatorname{sech}^2(x)\psi(x) = E\psi(x)$$

which is

$$-\psi''(x) - 2\operatorname{sech}^{2}(x)\psi(x) = \varepsilon\psi(x) \quad (*)$$

where $\varepsilon = 2mE/\hbar^2$.

$$A^{\dagger}A\psi = A^{\dagger} \left[\psi'(x) + \tanh(x)\psi(x) \right]$$

$$= -\psi''(x) - \operatorname{sech}^{2}(x)\psi(x) - \tanh(x)\psi'(x) + \tanh(x)\psi'(x) + \tanh^{2}(x)\psi(x)$$

$$= -\psi'' - 2\operatorname{sech}^{2}(x)\psi + \psi \qquad \text{using } \tanh^{2}(x) = 1 - \operatorname{sech}^{2}(x)$$

Hence, adding $\psi(x)$ to both sides of (*) it is rewritten as

$$A^{\dagger}A\psi = (\varepsilon + 1)\psi$$