PX2132 Introductory Quantum Mechanics Problems

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You have the videos, notes, and textbooks to help you. All videos are available on the youtube channel *Introductory Quantum Mechanics*, and links to videos, notes, and textbooks are available at felixflicker.com/teaching, or on Learning Central.

Each question is worth 20 marks. The exam will consist of five such questions, of which you must choose 4 to answer (80 marks total), for which you will have 2 hours. The number of marks is provided to give an idea of how long should be spent on each question.

For each question, a similar question with a worked solution is provided. The questions are designed to match the exam closely.

Satisfactory completion of each week's problem set is worth **2% of your total mark** for the course.

Satisfactory completion is defined as follows: for each mark within of the question, EITHER you make an attempt (which need not be successful) OR you write answers to the following:
(i) What didn't you understand which led you to get stuck?
(ii) Which textbook sections did you deem to be closest to what you needed? List at least 2 books.
(iii) How did these sections fall short?

Questions should be submitted via turnitin by the specified date.

Mark scheme

Worked examples include an indication of the style of question being asked, using letters A-G. The scheme is used when designing exam questions to ensure a balance of question types (you do not see the letters in the exam). The meanings are as follows.

(A) simple recollection from notes

(B) from notes but requires pulling together knowledge from across the course

(C) calculation similar to one seen in class

(D) derivation worked through in lectures

(E) derivation discussed but not worked through

(F) familiar concepts in an unseen situation

(G) unseen extension to concepts from lectures

1 The Motivation for Quantum Mechanics

1.0 Videos

There is no problem set this week. Please watch videos: **V1.0, V1.1, V1.2, V1.3, V1.4, V1.5**.

2 Scattering and tunnelling

Please hand in answers via turnitin no later than **2pm Monday week 2 (10th October)**.

2.0 Videos

Please watch videos: **V2.1a, V2.1b, V2.1c, V2.1d, V2.2, V2.3**.

2.1 Worked example

Consider the potential

$$V(x) = \begin{cases} 0,\ x < -L\,(\text{region 1}) \\ V_0,\ -L \le x \le L\,(\text{region 2}) \\ 0,\ x \ge L\,(\text{region 3}). \end{cases} \tag{1}$$

Assume the energy of the particle $E > V_0$, and that a wave is incident from the left ($x = -\infty$). Define the solutions to the time independent Schrodinger equation (TISE) in each region to be

$$\phi_1 = \exp(ikx) + r\exp(-ikx) \tag{2}$$

$$\phi_2 = a\exp(ik'x) + b\exp(-ik'x) \tag{3}$$

$$\phi_3 = t\exp(-ikx). \tag{4}$$

(i) Sketch the potential.

[2 marks,C]

(ii) State the TISE in terms of $V(x)$.

[1 mark,A]

(iii) Use the TISE to find k and k' in terms of E and V_0.

[4 marks,D]

(iv) State the two boundary conditions at each end of the barrier.

[4 marks,A]

(v) What is meant by 'resonant transmission'?

[1 mark,A]

(vi) Solving for the transmission probability gives the result

$$T = \frac{4E(E - V_0)}{4E(E - V_0) + V_0^2\sin^2\left(L\sqrt{2m(E - V_0)}/\hbar\right)}. \tag{5}$$

For which energies is the barrier at resonance?

[3 marks,E]

(vii) Show that the resonant transmission condition in this case is that $k'L = n\pi$ for positive integer n.

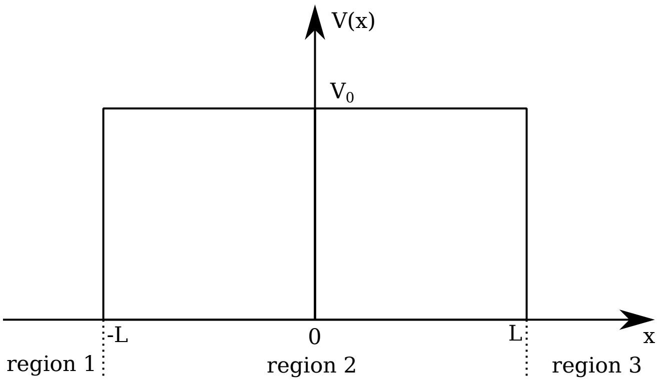
[2 marks,E]

(viii) Use the result of (vii) to sketch the wavefunctions of the two lowest-energy resonant states, marking on any key points.

[3 marks,G]

Answers to 2.1

(i)



- correct shape **[1 mark]**
- axis labels for L,$-L$, V_0 **[1 mark]**.
- No marks are available for labelling the three regions, but it is helpful to do so, and if you make errors later based on misunderstanding which region is which, marks can carry through from this earlier error if it's made clear.

(ii)

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi(x)}{\partial x^2}+V(x)\phi(x)=E\phi(x). \tag{6}$$

(iii) In region 1, TISE takes the form:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi_1(x)}{\partial x^2}=E\phi_1(x). \tag{7}$$

[1 mark].
Substitute the stated form to find:

$$\frac{\hbar^2k^2}{2m}\phi_1(x)=E\phi_1(x) \tag{8}$$

and therefore

$$\frac{\hbar^2k^2}{2m}=E \tag{9}$$

and

$$k=\frac{\sqrt{2mE}}{\hbar}. \tag{10}$$

[1 mark].

In region 2, TISE takes the form:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi_2(x)}{\partial x^2} + V_0\phi_2(x) = E\phi_2(x)\,. \tag{11}$$

Substitute the stated form of $\phi_2(x)$ to find

$$\frac{\hbar^2 k'^2}{2m}\phi_2(x) + V_0\phi_2(x) = E\phi_2(x) \tag{12}$$

[1 mark] and therefore

$$\frac{\hbar^2 k'^2}{2m} + V_0 = E \tag{13}$$

and

$$k' = \frac{\sqrt{2m(E - V_0)}}{\hbar} \tag{14}$$

[1 mark].

(iv) These are the two general boundary conditions which always apply: the wavefunction is continuous, and its first derivative is continuous except at infinite discontinuities in potential. This gives two conditions at each end of the barrier:

- $\phi_1(-L) = \phi_2(-L)$ **[1 mark]**
- $\phi_1'(-L) = \phi_2'(-L)$ **[1 mark]**
- $\phi_1(L) = \phi_2(L)$ **[1 mark]**
- $\phi_1'(L) = \phi_2'(L)$ **[1 mark].**

(v) Resonant transmission is when the probability for transmission is equal to 1. **[1 mark]**

(vi) Using the expression and the answer to (v), we require that

$$T = 1 = \frac{4E(E - V_0)}{4E(E - V_0) + V_0^2 \sin^2\left(L\sqrt{2m(E - V_0)}/\hbar\right)} \tag{15}$$

[1 mark]. Rearranging gives

$$\sin^2\left(L\sqrt{2m(E - V_0)}/\hbar\right) = 0 \tag{16}$$

[1 mark]. This is true whenever

$$E = V_0 + \frac{1}{2m}\left(\frac{n\pi\hbar}{L}\right)^2 \tag{17}$$

where n is any positive integer **[1 mark]**.

(vii) Now combine the results of (vi) and (iii). From Eq. 13

$$E - V_0 = \frac{\hbar^2 k'^2}{2m} \tag{18}$$

and substituting into Eq. 17 gives

$$\frac{\hbar^2 k'^2}{2m} = \frac{1}{2m}\left(\frac{n\pi\hbar}{L}\right)^2 \tag{19}$$

[1 mark] or

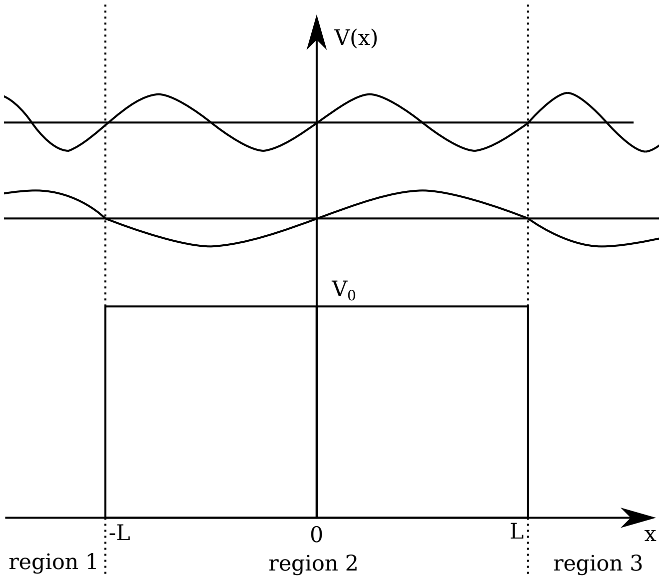
$$k'L = n\pi \tag{20}$$

as required **[1 mark].**

(viii) This question is a bit harder, to differentiate the top students. In general such questions may not have been discussed directly in class. It is perhaps easiest to think in terms of wavelengths using $\lambda' = 2\pi/k'$. Then the resonance condition is that

$$\lambda' = \frac{2L}{n} \tag{21}$$

and hence an integer number of wavelengths must fit along the barrier length of $2L$ **[1 mark]**. These are the results for $n = 1$ and $n = 2$.



A decent sketch with the zeroes marked on gives **[1 mark]**. NB there is no reflected wave, making the sketch simpler. You don't strictly need to show the waves above the barrier, as this is just a shorthand (really the real parts of the wavefunctions, shown here, have their own y-axes, but it is conventional to draw them on the potential plot like this).

Finally, note that the wavelength must be smaller in regions 1 and 3 than region 2, as the particle's energy has not had the barrier energy subtracted from it in these regions **[1 mark]**. I didn't draw this well on inkscape: note that the wavefunction and its derivative must still be continuous everywhere.

2.2 Question

A particle is incident from the left ($x = -\infty$) on a potential step defined by

$$V(x) = \begin{cases} 0, \, x < 0 \, (\text{region } I) \\ V_0, \, x \geq 0 \, (\text{region } II). \end{cases} \tag{22}$$

(i) Sketch the potential.

[2 marks]

(ii) State the TISE in terms of $V(x)$.

[1 mark]

(iii) Assuming $E < V_0$ explain why the solutions to the TISE take the forms

$$\phi_I(x) = \exp(ikx) + r\exp(-ikx) \tag{23}$$

$$\phi_{II}(x) = t\exp(-\kappa x). \tag{24}$$

[3 marks]

(iv) Using the TISE, find expressions for k and κ in terms of E and V_0.

[3 marks]

(v) State the two boundary conditions obeyed at the step.

[2 marks]

(vi) Find the reflection (r) and transmission (t) amplitudes in terms of k and κ.

[5 marks]

(vii) Sketch the waves in each region, paying attention to the amplitude, phase, and wavelength of the waves, for the case that $E \ll V_0$.

[4 marks]

3 Bound states

Please hand in answers via turnitin no later than **2pm Monday week 3 (17th October)**.

3.0 Videos

Please watch videos: **V3.1, V3.2, V3.3.**

3.1 Worked Example

Consider the TISE

$$\left(-\frac{\hbar^2}{2m}\partial_x^2 + V(x)\right)\phi_n(x) = E_n\phi_n(x) \tag{25}$$

with the potential

$$V(x) = \begin{cases} 0, & -L/2 \leq x \leq L/2 \\ \infty, & \text{otherwise.} \end{cases} \tag{26}$$

(i) Sketch the potential and the first four energy eigenfunctions.

[3 marks, D]

(ii) Explain which eigenfunctions $\phi_n(x)$ will be odd functions, and which even.

[2 marks, F]

(iii) Find the eigenvalues E_n and normalized eigenfunctions $\phi_n(x)$. Note that you will get different forms for the odd and even functions.

[7 marks, D]

(iv) Why do you not need to worry about the complex phase?

[1 mark, B]

(v) A particle in the well is in the first excited state, $\phi_2(x)$. What is the probability for it to be found in the region $x > L/4$?

[3 marks, B]

(vi) Now consider the finite potential well with the potential

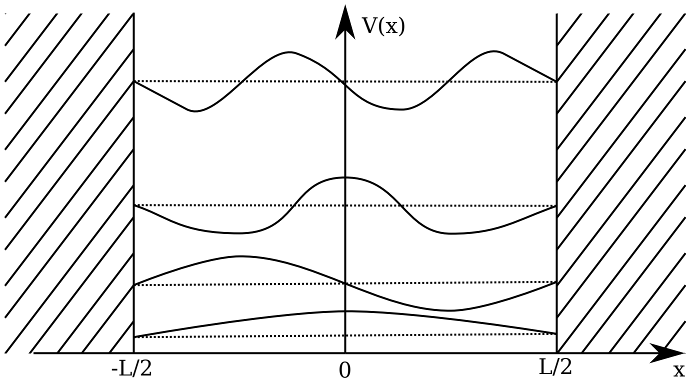
$$V(x) = \begin{cases} 0, & -L/2 \leq x \leq L/2 \\ V_0, & \text{otherwise.} \end{cases} \tag{27}$$

Stating any assumptions, give a rough estimate of the smallest value of V_0 for which $\phi_2(x)$ remains a bound state.

[4 marks, G]

Answers to 3.1

(i)



Sketch of potential, indicating forbidden regions **[1 mark]**; Correct axis labels x, $V(x)$, $\pm L/2$ **[1 mark]**; wavefunction sketches **[2 marks]**. Note that if the sketches are hard to read, marks can still be awarded provided key points are indicated. In this case this would be some written explanation of the locations of zeroes of the wavefunctions. NB the process of drawing the wavefunctions offset vertically on the same axis as the potential is common but misleading, and no marks would be lost if the wavefunctions were instead plotted separately. In any case, these are the real parts of the wavefunctions drawn at a specific time (two arbitrary choices).

(ii)

An odd function obeys $f(-x) = -f(x)$, while an even function obeys $f(-x) = f(x)$ **[1 mark]**. Hence, numbering the ground state $n = 1$, all odd n are even functions, and all even n are odd functions **[1 mark].** NB if you think this fact will prove important later, you're correct!

(iii)

Getting to the solution is a matter of guessing a form (making an ansatz) and confirming it solves the TISE, before normalizing. Based on the previous answers we can see that:

$$\phi_n(x) = \begin{cases} a_n \cos(k_n x), \; n \text{ odd} \\ b_n \sin(k_n x), \; n \text{ even.} \end{cases} \tag{28}$$

[1 mark]. Confirm both solve the TISE (inside the well, $V(x) = 0$):

$$-\frac{\hbar^2}{2m}\phi_n'' = E\phi_n \tag{29}$$

$$\downarrow$$

$$\frac{\hbar^2 k_n^2}{2m} = E_n \tag{30}$$

yes, they both work, and once we have k_n we also have the energy eigenvalues **[1 mark]**. Now we need to constrain k_n using the boundary conditions. In this case the conditions are that

$$\phi_n\left(x=-L/2\right)=\phi_n\left(x=L/2\right)=0 \tag{31}$$

[1 mark]. We have effectively used one boundary condition to specify that our functions are odd or even. Therefore just use one more condition to find k_n:

$$\phi_n\left(L/2\right)=0 \tag{32}$$

$$\downarrow$$

$$a_n\cos\left(k_nL/2\right)=0 \tag{33}$$

$$b_n\sin\left(k_nL/2\right)=0 \tag{34}$$

therefore

$$k_n=n\pi/L \tag{35}$$

for both odd and even **[1 mark]**. Hence from Eq. 30 we have the energy eigenvalues

$$E_n=\frac{\hbar^2n^2\pi^2}{2mL^2} \tag{36}$$

[1 mark]. Finally, we need the normalizations. Since the particle must exist somewhere in the well, the probability to find it across the entire well must be one:

$$\int_{-L/2}^{L/2}\left|\phi_n\right|^2\mathrm{d}x=1 \tag{37}$$

[1 mark]. Hence

$$\left|a_n\right|^2\int_{-L/2}^{L/2}\cos^2\left(k_nx\right)\mathrm{d}x=1$$

and using

$$\cos^2\left(x\right)+\sin^2\left(x\right)=1 \tag{38}$$

$$\cos^2\left(x\right)-\sin^2\left(x\right)=\cos\left(2x\right) \tag{39}$$

we get

$$\begin{aligned} |a_n|^2 \int_{-L/2}^{L/2} \frac{1+\cos(2k_n x)}{2} \mathrm{d}x &= 1 \\ |a_n|^2 \frac{L}{2} &= 1 \\ |a_n| &= \sqrt{\frac{2}{L}}. \end{aligned}$$

Similarly for the odd n case:

$$\begin{aligned} |b_n|^2 \int_{-L/2}^{L/2} \sin^2(k_n x)\, \mathrm{d}x &= 1 \\ |b_n|^2 \int_{-L/2}^{L/2} \frac{1-\cos(2k_n x)}{2} \mathrm{d}x &= 1 \\ |b_n|^2 \frac{L}{2} &= 1 \\ |b_n| &= \sqrt{\frac{2}{L}}. \end{aligned}$$

[1 mark] in total for the normalization calculations (this might seem a bit stingy, but it's all standard bookwork). Putting it all together makes it easier for the marker, and hence less likely anything will be missed:

$$\phi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right), \, n \text{ odd} \\ \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \, n \text{ even} \end{cases} \tag{40}$$

and

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}. \tag{41}$$

(iv)
The global phase is unobservable in quantum mechanics. It is a redundancy of the mathematics we use to describe the problem: only relative phases can be measured. (A comment along any of these lines receives the mark).
(v) Using the Born Rule the probability is

$$P = \int_{L/4}^{L/2} |\phi_2(x)|^2 \, \mathrm{d}x \tag{42}$$

[1 mark]. Therefore

$$P = \frac{2}{L}\int_{L/4}^{L/2} \sin^2\left(\frac{2\pi x}{L}\right) \mathrm{d}x \tag{43}$$

[1 mark] and

$$\begin{aligned} P &= \frac{1}{L}\int_{L/4}^{L/2} \left(1 - \cos\left(4\pi x/L\right)\right) \mathrm{d}x \\ &= \frac{1}{4} - \left[\frac{L}{4\pi}\sin\left(4\pi x/L\right)\right]_{L/4}^{L/2} \\ &= \frac{1}{4}. \end{aligned}$$

[1 mark]. If a solid argument is provided in words to explain why the result must be 1/4 based on the form of the wavefunction, this can receive full marks without the working.

(vi) This is a difficult question to differentiate the top few students. Getting all the marks will be hard, but there are book marks available along the way for setting up the problem.

Call the left barrier region I, the well region II, and the right barrier III. Our ansatz for the odd wavefunctions is

$$\phi_I = A\exp\left(\kappa x\right) \tag{44}$$

$$\phi_{II} = B\sin\left(k_n x\right) \tag{45}$$

$$\phi_{III} = -A\exp\left(-\kappa x\right) \tag{46}$$

(a sketch would help get you the marks here if there are any errors). **[1 mark]** for setting up the problem correctly; the reasoning could be based on the forms of the infinite well solutions just obtained, or the full method from the notes could be used.

From the TISE we have

$$-\frac{\hbar^2\kappa^2}{2m} + V_0 = E \tag{47}$$

$$\frac{\hbar^2 k_n^2}{2m} = E. \tag{48}$$

Finally, we need to use our boundary conditions, say at the region II to III boundary:

$$\phi_{II}\left(L/2\right) = \phi_{III}\left(L/2\right) \tag{49}$$
$$\phi'_{II}\left(L/2\right) = \phi'_{III}\left(L/2\right) \tag{50}$$

giving

$$B\sin\left(k_n L/2\right) = -A\exp\left(-\kappa L/2\right) \tag{51}$$
$$-Bk_n\cos\left(k_n L/2\right) = A\kappa\exp\left(-\kappa L/2\right). \tag{52}$$

Dividing the last two equations gives

$$\frac{\tan\left(k_n L/2\right)}{k_n} = \frac{1}{\kappa}. \tag{53}$$

Now substitute the expressions for κ and k_n in terms of E and V_0 :

$$\hbar\frac{\tan\left(\frac{\sqrt{2mE}L}{2\hbar}\right)}{\sqrt{2mE}} = \frac{\hbar}{\sqrt{2m\left(V_0 - E\right)}} \tag{54}$$

and re-arrange:

$$\tan^2\left(\frac{\sqrt{2mE}L}{2\hbar}\right) = \frac{E}{V_0 - E} \tag{55}$$
$$\downarrow \tag{56}$$
$$\frac{E}{V_0} = \sin^2\left(\frac{\sqrt{2mE}L}{2\hbar}\right) \tag{57}$$

[1 mark] for result, **[1 mark]** for working. We want a solution for the smallest value of V_0, and so we need the smallest value of $\frac{\sqrt{2mE}L}{2\hbar}$ which gives a solution. Assuming $\frac{\sqrt{2mE}L}{2\hbar}$ is small, we can expand the sine to give

$$\frac{E}{V_0} \approx \frac{mEL^2}{2\hbar^2} \tag{58}$$

and so

$$V_0 \approx \frac{2\hbar^2}{mL^2} \tag{59}$$

[1 mark]. Following the notes, a sketch of E/V_0 and $\sin^2\left(\frac{\sqrt{2mE}L}{2\hbar}\right)$ plotted on the same axes makes it clear why V_0 requires a minimum value for solutions to exist. Correct graphical arguments can give up to 2 marks without a correct answer.

3.2 Question

Consider the TISE

$$\left(-\frac{\hbar^2}{2m}\partial_x^2 + V(x)\right)\phi_n(x) = E_n\phi_n(x) \tag{60}$$

with the potential

$$V(x) = \begin{cases} 0, & 0 \le x \le L \\ \infty, & \text{otherwise.} \end{cases} \tag{61}$$

(i) Sketch the potential and the first four energy eigenfunctions.

[3 marks]

(ii) Find the eigenvalues E_n and normalized eigenfunctions $\phi_n(x)$.

[7 marks]

(iii) A particle is found to have energy E_n. Find the probability for it to exist in the region $0 \le x \le \alpha L$ where $0 \le \alpha \le 1$.

[3 marks]

(iv) Explain the probabilities you find at $\alpha = 0$, $1/2$, and 1.

[3 marks]

(v) Sketch the probability as a function of α for $n = 1$, marking on key points.

[2 marks]

(vi) Now consider the finite potential well defined by

$$V(x) = \begin{cases} 0, & 0 \le x \le L \\ V_0, & \text{otherwise.} \end{cases} \tag{62}$$

Explain whether the probability to exist in the region $0 \le x \le \alpha L$ where $0 \le \alpha \le 1$ increases or decreases compared to the infinite well case.

[2 marks]

4 Quantum Superposition

Please hand in answers via turnitin no later than **2pm Monday week 4 (24th October)**.

4.0 Videos

Please watch videos: **V4.1, V4.2, V4.3, V4.4**

4.1 Worked Example

(i) Explain why energy eigenstates are also called stationary states.

[2 marks, A]

(ii) Show that a superposition of two energy eigenstates with different energies cannot be a stationary state.

[3 marks, C]

(iii) Explain why any function $f(x)$ matching the same boundary conditions as the energy eigenstates $\phi_n(x)$ can be written as

$$f(x) = \sum_n^\infty f_n \phi_n(x) \tag{63}$$

by finding an expression for the coefficients f_n.

[5 marks, D]

(iv) Consider the infinite potential well

$$V(x) = \begin{cases} 0, & -L/2 \le x \le L/2 \\ \infty, & \text{otherwise} \end{cases} \tag{64}$$

which has energy eigenstates

$$\phi_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right), \; n \text{ odd} \\ \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \; n \text{ even} \end{cases} \tag{65}$$

for integer $n > 0$ and energy eigenvalues

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}. \tag{66}$$

A state is prepared whose wavefunction takes the form

$$g(x) = \begin{cases} -A, & -L/4 \le x < 0 \\ A, & 0 < x \le L/4 \\ 0, & \text{otherwise.} \end{cases} \tag{67}$$

Find A such that the state $g(x)$ is correctly normalized.

[2 marks, C]

(v) Explain why, if a measurement of energy is made, the probability to find energy E_{2n+1} is zero.

[4 marks, B]

(vi) Find the subsequent time evolution $g(x,t)$.

[4 marks, C]

Answers to 4.1

(i) The time dependence of an energy eigenstate appears only as a complex phase:

$$\psi_n(x,t) = \phi_n(x)\exp(-iE_n t/\hbar) \tag{68}$$

[1 mark]. Hence the probability density of an energy eigenstate is independent of time:

$$|\psi_n(x,t)|^2 = |\phi_n(x)|^2 \tag{69}$$

[1 mark].

(ii) A superposition of two energy eigenstates takes the form

$$\frac{1}{\sqrt{2}}\left(\psi_n(x,t) + \psi_m(x,t)\right) \tag{70}$$

with $n \neq m$ **[1 mark]** and therefore

$$\frac{1}{\sqrt{2}}\left(\phi_n(x)\exp(-iE_n t/\hbar) + \phi_m(x)\exp(-iE_m t/\hbar)\right). \tag{71}$$

The probability density $\rho(x,t)$ is therefore

$$\rho = \frac{1}{2}\left|\phi_n(x)\exp(-iE_n t/\hbar) + \phi_m(x)\exp(-iE_m t/\hbar)\right|^2 \tag{72}$$

and so

$$\frac{1}{2}|\phi_n(x)|^2 + \frac{1}{2}|\phi_m(x)|^2 + \mathfrak{Re}\left[\phi_n(x)\phi_m^*(x)\exp\left(-i(E_n - E_m)t/\hbar\right)\right] \tag{73}$$

[1 mark]. The final term is time dependent because $E_n \neq E_m$ **[1 mark]**.

(iii) Energy eigenstates form a complete orthonormal basis **[1 mark]**. By definition this means that any function matching the same boundary conditions can be written as a linear combination of these states. Mathematically,

$$\int_{-\infty}^{\infty} \phi_n^*(x)\,\phi_m(x)\,\mathrm{d}x = \delta_{nm} \tag{74}$$

where

$$\delta_{nm} = \begin{cases} 1, & n = m \\ 0, & n \neq m \end{cases} \tag{75}$$

[1 mark]. To show that we can write

$$f(x) = \sum_{n}^{\infty} f_n \phi_n(x) \tag{76}$$

we just need to show that we have solutions for f_n. To do this, work backwards:

$$f(x) = \sum_{n}^{\infty} f_n \phi_n(x) \tag{77}$$

$$\downarrow$$

$$\int_{-\infty}^{\infty} \phi_m^*(x) f(x)\, \mathrm{d}x = \int_{-\infty}^{\infty} \phi_m^*(x) \sum_{n}^{\infty} f_n \phi_n(x)\, \mathrm{d}x \tag{78}$$

$$= \sum_{n}^{\infty} f_n \int_{-\infty}^{\infty} \phi_m^*(x)\, \phi_n(x)\, \mathrm{d}x \tag{79}$$

$$= \sum_{n}^{\infty} f_n \delta_{nm} \tag{80}$$

$$= f_m \tag{81}$$

[2 marks]. Hence, changing labels from m to n, we have

$$f_n = \int_{-\infty}^{\infty} \phi_n^*(x)\, f(x)\, \mathrm{d}x \tag{82}$$

[1 mark]. Any reasonable statement as to *why* it should work (the eigenfunctions form an orthonormal basis for the infinite dimensional Hilbert space of L^2 normalizable functions matching the boundary conditions) can give up to 2 marks in the absence of a correct numerical answer.

(iv) We require

$$\int_{-\infty}^{\infty} |g(x)|^2\, \mathrm{d}x = 1 \tag{83}$$

and so

$$\int_{-L/4}^{L/4} |A|^2\, \mathrm{d}x = 1$$

[1 mark] requiring

$$|A| = \sqrt{\frac{2}{L}} \tag{84}$$

[1 mark].

(v) The function $g(x)$ is odd, meaning $g(-x) = -g(x)$. Therefore any even eigenstates cannot contribute to the sum **[1 mark]**. The odd-numbered energy eigenstates, with energies E_{2n+1}, are even functions, and hence do not contribute **[1 mark]**. The probability to measure energy E_{2n+1} is given by the square modulus of the corresponding coefficient in the superposition, g_{2n+1} **[1 mark]**. But we've just argued that these coefficients are all zero, and hence there is zero probability to measure the energy E_{2n+1} **[1 mark]**.

(vi) Writing

$$g(x) = \sum_{n=1}^{\infty} g_n \phi_n(x) \tag{85}$$

the subsequent time evolution is

$$g(x,t) = \sum_{n=1}^{\infty} g_n \phi_n(x) \exp\left(-iE_n t/\hbar\right) \tag{86}$$

$$g(x,t) = \sum_{n=1}^{\infty} g_n \phi_n(x) \exp\left(-i\frac{\hbar^2 n^2 \pi^2 t}{2mL^2\hbar}\right) \tag{87}$$

[1 mark]. We therefore need the coefficients g_n, which we showed are given by

$$g_n = \int_{-\infty}^{\infty} \phi_n^*(x)\, g(x)\, \mathrm{d}x. \tag{88}$$

We have just explained that $g_{n\,\mathrm{odd}} = 0$ **[1 mark]**. For the rest we have

$$\begin{aligned}
g_{n\,\mathrm{even}} &= -\int_{-L/4}^{0} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \sqrt{\frac{2}{L}} \mathrm{d}x + \int_{0}^{L/4} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \sqrt{\frac{2}{L}} \mathrm{d}x \\
&= \frac{4}{L} \int_{0}^{L/4} \sin\left(\frac{n\pi x}{L}\right) \mathrm{d}x \\
&= \frac{4}{n\pi} \left[\cos\left(\frac{n\pi x}{L}\right)\right]_0^{L/4} \\
&= \frac{4}{n\pi} \left[\cos\left(\frac{n\pi}{4}\right) - 1\right]
\end{aligned}$$

[1 mark]. Therefore

$$g\left(x,t\right)=\sqrt{\frac{2}{L}}\sum_{n\,\mathrm{even}}\frac{4}{n\pi}\left[\cos\left(\frac{n\pi}{4}\right)-1\right]\sin\left(\frac{n\pi x}{L}\right)\exp\left(-i\frac{\hbar^2n^2\pi^2t}{2mL^2\hbar}\right) \tag{89}$$

[1 mark]. This can be rewritten by noting that the cosine only takes the values ±1, 0, although there's no real simplification in doing so.

4.2 Question

(i) Show that the probability density

$$\rho(x) = |\psi_n(x,t)|^2 \tag{90}$$

is time independent for all energy eigenfunctions.

[1 mark]

(ii) Now consider the superposition

$$\chi(x,t) = \alpha\psi_1(x,t) + \beta\psi_2(x,t) \tag{91}$$

where α and β are complex numbers. Find a condition on α and β such that χ is properly normalized.

[4 marks]

(iii) For the special case that ϕ_1, ϕ_2, α and β are all real, show that the probability density

$$\rho_\chi(x) = |\chi(x,t)|^2 \tag{92}$$

is now time dependent, and find an expression for the period.

[4 marks]

(iv) Consider the infinite potential well

$$V(x) = \begin{cases} 0, & -L/2 \leq x \leq L/2 \\ \infty, & \text{otherwise} \end{cases} \tag{93}$$

which has energy eigenstates

$$\phi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right), & n \text{ odd} \\ \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), & n \text{ even} \end{cases} \tag{94}$$

for integer $n > 0$. Explain why the expectation value of position is zero for every state.

[3 marks]

(v) Find the standard deviation of the position

$$\sigma_{\hat{x}} = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2} \tag{95}$$

for each state.

[5 marks]

(vi) Your experimentalist friend intends to measure the average position of the particle in its ground state. State the expected result including an estimate of the error.

[3 marks]

5 Finite-dimensional Hilbert spaces

Please hand in answers via turnitin no later than **2pm Monday week 5 (31st October)**. [Note: problem set 6 is also due this week]

5.0 Videos

Please watch videos: **V5.1, V5.2, V5.3a, V5.3b, V5.3c, V5.4.**

5.1 Worked Example

(i) Prove that Hermitian matrices have real eigenvalues.

[4 marks, A]

(ii) A Stern Gerlach apparatus is used to identify that a silver atom has spin-up along the z-direction. For each of the following measurements, state the possible outcomes and their probabilities.

(a) A measurement of spin along the x-direction.

[2 marks, B]

(b) A measurement of spin along the y-direction.

[2 marks, B]

(c) A measurement of spin along the z-direction.

[2 marks, B]

(iii) Consider the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{96}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{97}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{98}$$

Define the spin operators

$$\hat{S}_i = \frac{\hbar}{2}\sigma_i \tag{99}$$

for $i \in \{x, y, z\}$. Given this definintion, explain why the states corresponding to spin-up and spin-down along x must then take the form

$$|\uparrow_z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow_z\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{100}$$

[3 marks, D]

(iv) State the equivalent expressions for $|\uparrow_x\rangle$ and $|\downarrow_x\rangle$.

[3 marks, D]

(v) Show that the operators $\hat{S}_x$ and $\hat{S}_z$ do not commute.

[2 marks, C]

(vi) Explain what this means physically in terms of repeated Stern Gerlach measurements and their possible outcomes.

[2 marks, F]

Answers to 5.1

(i) Denote the eigenvector with eigenvalue λ_n by $|n\rangle$:

$$M|v_n\rangle = \lambda_n|v_n\rangle. \tag{101}$$

Taking the Hermitian conjugate we have

$$\begin{gathered}(M|v_n\rangle)^\dagger = (\lambda_n|v_n\rangle)^\dagger \\ \downarrow \\ \langle v_n|M^\dagger = \langle v_n|\lambda_n^*\end{gathered} \tag{102}$$

[1 mark].
Therefore

$$\langle v_n|M - M^\dagger|v_n\rangle = (\lambda_n - \lambda_n^*)\,\langle v_n|v_n\rangle \tag{103}$$

because we can act right with M using Eq. 101 and left with $M^\dagger$ using Eq. 102 **[1 mark]**.
Since

$$\langle v_n|v_n\rangle > 0 \tag{104}$$

[1 mark] we see that

$$M = M^\dagger \Rightarrow \lambda = \lambda^* \tag{105}$$

i.e. Hermitian operators have real eigenvalues **[1 mark]**.
(ii)
(a) spin-up along x, probability $1/2$ **[1 mark]**, and spin-down along x, probability $1/2$ **[1 mark]**.
(b) spin-up along y, probability $1/2$ **[1 mark]**, and spin-down along y, probability $1/2$ **[1 mark]**.
(c) spin-up along z is the only possibility, with probability 1 **[2 marks]**.
Just stating “spin-up” (etc) without stating the direction can receive at most half marks.
(iii) In quantum mechanics observable quantities are encoded in Hermitian operators; the possible outcomes of measurements are the eigenvalues of those operators. Here we require that

$$\hat{S}_z|\uparrow_z\rangle = \frac{\hbar}{2}|\uparrow_z\rangle \tag{106}$$
$$\hat{S}_z|\downarrow_z\rangle = -\frac{\hbar}{2}|\downarrow_z\rangle \tag{107}$$

[1 mark]. Given that

$$\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{108}$$

we therefore require

$$|\uparrow_z\rangle \propto \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow_x\rangle \propto \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{109}$$

since

$$\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{110}$$
$$\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{111}$$

[1 mark]. We also require the states to be normalised, as the total probability to obtain some outcome from a measurement is 1. Therefore the proportionality signs in Eq. 109 become equalities **[1 mark]**.

(iv)

$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |\downarrow_x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{112}$$

[1 mark] for vectors, **[1 mark]** for normalisation. These can be found by the usual method of finding eigenvectors, or simply by trying some obvious cases. In either case, show that they work as planned:

$$\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{113}$$

$$\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{114}$$

[1 mark].

(v)

$$\left[\hat{S}_x, \hat{S}_z\right] = \frac{\hbar^2}{4}\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] \tag{115}$$

[1 mark] and

$$\left[\hat{S}_x, \hat{S}_z\right] = \frac{\hbar^2}{4}\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] \tag{116}$$

$$= \frac{\hbar^2}{4}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{117}$$

$$= \frac{\hbar^2}{4}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} - \frac{\hbar^2}{4}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{118}$$

$$= \frac{\hbar^2}{2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{119}$$

which is not zero **[1 mark]**.

(vi) The previous result tells us that the observables corresponding to the operators cannot be known simultaneously **[1 mark]**. Therefore, measuring spin along x, a subequent measurement of spin along z must return an indeterminate answer (a finite probability for either outcome). Similarly for any measurement along z followed by a measurement along x; **[1 mark]** for any statement to this effect.

5.2 Question

(i) Assuming the eigenvalues of a Hermitian matrix are non-degenerate, prove that the corresponding eigenvectors are orthogonal.

[4 marks]

(ii) Consider the spin matrices

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{120}$$

State three properties which make them appropriate as a choice of operators to encode spin-1/2.

[3 marks]

(iii) In this basis, explain why the states corresponding to spin-up and spin-down along y must then take the form

$$|\uparrow_y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}, \quad |\downarrow_y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}. \tag{121}$$

[2 marks]

(iv) State the equivalent forms for $|\uparrow_z\rangle$ and $|\downarrow_z\rangle$.

[1 mark]

(v) Hence express $|\uparrow_z\rangle$ as a linear combination of $|\uparrow_y\rangle$ and $|\downarrow_y\rangle$.

[3 marks]

(vi) A Stern Gerlach apparatus is used to establish that a spin-1/2 silver atom has spin up along z. The same atom then passes through a second Stern Gerlach apparatus oriented so as to perform a measurement of the spin along y. Using your previous result, calculate the probability that the outcome is spin up along y.

[3 marks]

(vii) Rather than record the outcome of the second measurement, the two possible routes are redirected so as to rejoin one another, and the resulting route passes through a second Stern Gerlach apparatus so as to measure the spin along z. Calculate the probability that the outcome is spin up along z, and comment on any implications this may have regarding the nature of reality.

[4 marks]

6 Operators and observables

Please hand in answers via turnitin no later than **2pm Monday week 5 (31st October)**. [Note: same deadline as problem set 5]

6.0 Videos

Please watch videos: **V6.1, V6.2, V6.3, V6.4**.

6.1 Worked Example

(i) Explain what is meant by a good quantum number.

[2 marks, A]

(ii) Explain what is meant by the Heisenberg and Schrodinger pictures.

[2 marks, A]

(iii) Write an expression for an operator $\hat{A}_H(t)$ in the Heisenberg picture, in terms of the equivalent operator $\hat{A}_S$ in the Schroedinger picture.

[1 mark, A]

(iv) Write an expression for a state $|\psi_H\rangle$ in the Heisenberg picture, in terms of the equivalent state $|\psi_S(t)\rangle$ in the Schroedinger picture.

[1 mark, A]

(v) Using (iii) and (iv) show that

$$\langle\varphi_H|\hat{A}_H(t)|\psi_H\rangle = \langle\varphi_S(t)|\hat{A}_S|\psi_S(t)\rangle \tag{122}$$

and hence that the two pictures are equivalent.

[2 marks, C]

(vi) Derive the Heisenberg equation of motion:

$$i\hbar\frac{\mathrm{d}\hat{A}_H(t)}{\mathrm{d}t} = \left[\hat{A}_H(t), \hat{H}\right]. \tag{123}$$

[4 marks, C]

(vii) Use the previous results to prove Ehrenfest's theorem:

$$i\hbar\frac{\mathrm{d}\langle\hat{A}\rangle}{\mathrm{d}t} = \langle\left[\hat{A}, \hat{H}\right]\rangle. \tag{124}$$

[2 marks, C]

(viii) Explain why, if the operator describing an observable commutes with the Hamiltonian, then the observable corresponds to a good quantum number.

[2 marks, D]

(ix) Hence explain why energy is always a good quantum number.

[2 marks, D]

(x) Explain why it is always possible to have simultaneous knowledge of a quantum number and of the energy of the system.

[2 marks, F]

Answers to 6.1

(i) A good quantum number is an expectation value of an operator which is time independent. **[1 mark]**

For the observable represented by operator $\hat{Q}$ to be a good quantum number for a state $|\psi\rangle$, its expectation value must be conserved:

$$\frac{\mathrm{d}\langle\psi|\hat{Q}|\psi\rangle}{\mathrm{d}t} = 0 \tag{125}$$

[1 mark].

(ii) In the Heisenberg picture states are time-independent, but operators are time dependent **[1 mark].**

In the Schroedinger picture states are time-dependent but operators are time independent **[1 mark].**

(iii)

$$\hat{A}_H\left(t\right) = \exp\left(i\hat{H}t/\hbar\right)\hat{A}_S\exp\left(-i\hat{H}t/\hbar\right). \tag{126}$$

(iv)

$$|\psi_H\rangle = \exp\left(i\hat{H}t/\hbar\right)|\psi_S\left(t\right)\rangle \tag{127}$$

(up to a constant phase).

(v)

$$\langle\varphi_H|\hat{A}_H\left(t\right)|\psi_H\rangle = \langle\varphi_S\left(t\right)|\exp\left(-i\hat{H}t/\hbar\right)\hat{A}_H\left(t\right)\exp\left(i\hat{H}t/\hbar\right)|\psi_S\left(t\right)\rangle \tag{128}$$

[1 mark] and

$$\exp\left(-i\hat{H}t/\hbar\right)\hat{A}_H\left(t\right)\exp\left(i\hat{H}t/\hbar\right) = \hat{A}_S \tag{129}$$

so

$$\langle\varphi_H|\hat{A}_H\left(t\right)|\psi_H\rangle = \langle\varphi_S\left(t\right)|\hat{A}_S|\psi_S\left(t\right)\rangle \tag{130}$$

[1 mark]. Hence the two pictures are equivalent, and we can write $\left\langle\varphi|\hat{A}|\psi\right\rangle$ unambiguously.

(vi) Starting from

$$\hat{A}_H(t) = \exp\left(i\hat{H}t/\hbar\right)\hat{A}_S \exp\left(-i\hat{H}t/\hbar\right) \tag{131}$$

take the partial derivative with respect to time:

$$\frac{\partial \hat{A}_H(t)}{\partial t} = \frac{\partial}{\partial t}\left(\exp\left(i\hat{H}t/\hbar\right)\hat{A}_S \exp\left(-i\hat{H}t/\hbar\right)\right) \tag{132}$$

$$= \frac{i\hat{H}}{\hbar}\exp\left(i\hat{H}t/\hbar\right)\hat{A}_S \exp\left(-i\hat{H}t/\hbar\right) - \exp\left(i\hat{H}t/\hbar\right)\hat{A}_S \frac{i\hat{H}}{\hbar}\exp\left(-i\hat{H}t/\hbar\right) \tag{133}$$

[1 mark]. NB $\hat{A}_H$ and $\hat{H}$ need not commute, so be careful to get the order right in both terms. However, $\hat{H}$ and $\exp\left(-i\hat{H}t/\hbar\right)$ do always commute, as they're both just functions of $\hat{H}$. Therefore

$$\frac{\partial \hat{A}_H(t)}{\partial t} = \frac{i\hat{H}}{\hbar}\exp\left(i\hat{H}t/\hbar\right)\hat{A}_S \exp\left(-i\hat{H}t/\hbar\right) - \frac{i}{\hbar}\exp\left(i\hat{H}t/\hbar\right)\hat{A}_S \exp\left(-i\hat{H}t/\hbar\right)\hat{H} \tag{134}$$

$$= \frac{i}{\hbar}\hat{H}\hat{A}_H(t) - \frac{i}{\hbar}\hat{A}_H(t)\hat{H}$$

[1 mark]

$$= \frac{i}{\hbar}\left[\hat{H},\hat{A}_H(t)\right] \tag{135}$$

[1 mark]. Finally note that since $\hat{A}_H$ is only a function of time,

$$\frac{\partial \hat{A}_H(t)}{\partial t} = \frac{\mathrm{d}\hat{A}_H(t)}{\mathrm{d}t} \tag{136}$$

[1 mark] and so

$$\frac{\mathrm{d}\hat{A}_H(t)}{\mathrm{d}t} = \frac{i}{\hbar}\left[\hat{H},\hat{A}_H(t)\right]. \tag{137}$$

(vii)

$$i\hbar\frac{\mathrm{d}\hat{A}_H(t)}{\mathrm{d}t} = \left[\hat{A}_H(t),\hat{H}\right] \tag{138}$$

therefore

$$i\hbar\langle\psi_H|\frac{\mathrm{d}\hat{A}_H\left(t\right)}{\mathrm{d}t}|\psi_H\rangle = \langle\psi_H|\left[\hat{A}_H\left(t\right),\hat{H}\right]|\psi_H\rangle. \tag{139}$$

Since $|\psi_H\rangle$ is independent of time we can pull it inside the derivative:

$$i\hbar\frac{\mathrm{d}\langle\psi_H|\hat{A}_H\left(t\right)|\psi_H\rangle}{\mathrm{d}t} = \langle\psi_H|\left[\hat{A}_H\left(t\right),\hat{H}\right]|\psi_H\rangle. \tag{140}$$

[1 mark] Finally, recall that expectation values are independent of picture, so we can write

$$i\hbar\frac{\mathrm{d}\langle\psi|\hat{A}|\psi\rangle}{\mathrm{d}t} = \langle\psi|\left[\hat{A},\hat{H}\right]|\psi\rangle \tag{141}$$

or in the usual abbreviation

$$i\hbar\frac{\mathrm{d}\langle\hat{A}\rangle}{\mathrm{d}t} = \langle\left[\hat{A},\hat{H}\right]\rangle \tag{142}$$

[1 mark].

(viii) If an operator $\hat{Q}$ corresponds to a good quantum number then

$$\frac{\mathrm{d}\langle\hat{Q}\rangle}{\mathrm{d}t} = 0 \tag{143}$$

[1 mark].

From Ehrenfest's theorem this means that

$$\langle\left[\hat{Q},\hat{H}\right]\rangle = 0. \tag{144}$$

Therefore if $\hat{Q}$ commutes with $\hat{H}$ then $\frac{\mathrm{d}\langle\hat{Q}\rangle}{\mathrm{d}t} = 0$, and hence it is a good quantum number. **[1 mark]**

(ix) The operator corresponding to energy is the Hamiltonian **[1 mark]**.

Clearly, $\hat{H}$ commutes with itself. Therefore

$$\frac{\mathrm{d}\langle\hat{H}\rangle}{\mathrm{d}t} = 0. \tag{145}$$

[1 mark].

(x) The logic now works in reverse. If an observable is a good quantum number, its operator commutes with the Hamiltonian. But if two operators commute, they share a set of eigenvectors, and their eigenvalues can be known simultaneously. **[1 mark]** Hence, the quantum number and the energy (observable corresponding to the Hamiltonian operator) can be known simultaneously. **[1 mark]**

6.2 Question

(i) State the (generalised) Heisenberg uncertainty principle, explaining all terms.

[2 marks]

(ii) State the canonical commutation relation between position and momentum, explaining all terms.

[2 marks]

(iii) Use this to find the Heisenberg uncertainty relation between the position and momentum of a particle.

[3 marks]

(iv) Ehrenfest's theorem states that

$$i\hbar\frac{\mathrm{d}\langle\hat{A}\rangle}{\mathrm{d}t} = \langle\left[\hat{A},\hat{H}\right]\rangle \tag{146}$$

where $\hat{H}$ is the Hamiltonian. Find an expression for the product of the uncertainties between an observable A and the energy.

[1 mark]

(v) Using the definition of uncertainty you provided in (i), show that the uncertainty of an operator evaluated for an eigenvector of that operator is always zero.

[2 marks]

(vi) An operator $\hat{A}$ commutes with the Hamiltonian. State the minimum value of the product of the uncertainties in $\hat{A}$ and $\hat{H}$, and give an example of a state which gives this minimum value.

[4 marks]

(vii) Explain why the position operator can never commute with the Hamiltonian.

[2 marks]

(viii) Find the minimum value of the product of the uncertainties in $\hat{x}$ and $\hat{H}$, in terms of $\hat{p}$.

[4 marks]

7 Quantum mechanics

Please hand in answers via turnitin no later than **2pm Monday week 7 (14th November)**.

7.0 Videos

Please watch videos: **V7.1, V7.2, V7.3, V7.4, V7.5**.

7.1 Worked Example

(i) Give a mathematical expression for the normalisation of the wavefunction $\psi(x)$ and explain its physical meaning.

[2 marks, A]

(ii) The resolution of the identity can be written

$$\hat{\mathbb{I}} = \int_{-\infty}^{\infty} |x\rangle\langle x|\mathrm{d}x \tag{147}$$

where $|x\rangle$ is an eigenstate of the position operator $\hat{x}$:

$$\hat{x}|x\rangle = x|\hat{x}\rangle. \tag{148}$$

Defining the wavefunction $\psi(x) = \langle x|\psi\rangle$, use the normalisation of the wavefunction to derive the norm of the state $|\psi\rangle$.

[3 marks, C]

(iii) Working in the position basis, state the condition for a differential operator $\hat{A}$ to be Hermitian.

[2 marks, A]

(iv) State whether each of the following operators, written in the position basis, is Hermitian. If it is not, state its Hermitian conjugate.

(a) x

[1 mark, E]

(b) $-i\hbar\partial_x$

[1 mark, E]

(c) ∂_x

[1 mark, E]

(d) ∂_x^2

[1 mark, E]

(e) ∇

[1 mark, E]

(v) Show that the expectation value of an operator $\hat{A}$ in state $|\psi\rangle$, $\langle\psi|\hat{A}|\psi\rangle$, can be written in the position basis as

$$\langle\psi|\hat{A}|\psi\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi^*(x)\,A(x,y)\,\psi(y)\,\mathrm{d}x\mathrm{d}y \tag{149}$$

and give an expression for $A(x,y)$.

[4 marks, G]

(vi) Explain physically why we might expect

$$A(x,y) = A(x)\,\delta(x-y) \tag{150}$$

where $\delta(x-y)$ is the Dirac delta function.

[2 marks, G]

(vii) Hence, when Eq 150 is obeyed, show that

$$\langle\psi|\hat{A}|\psi\rangle = \int_{-\infty}^{\infty} \psi^*(x)\,A(x)\,\psi(x)\,\mathrm{d}x. \tag{151}$$

[2 marks, F]

Answers to 7.1

(i) The particle must exist somewhere in space, and so the integral of the probability density across all of space must equal one **[1 mark].**

Mathematically,

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, \mathrm{d}x = 1 \tag{152}$$

[1 mark].

(ii)

Since

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, \mathrm{d}x = 1 \tag{153}$$

we have

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,\mathrm{d}x & (154)\\ &= \int_{-\infty}^{\infty} \langle\psi|x\rangle\langle x|\psi\rangle \mathrm{d}x & (155) \end{aligned}$$

[1 mark]. The eigenstate $|\psi\rangle$ is independent of position, so

$$1 = \langle\psi| \left(\int_{-\infty}^{\infty} |x\rangle\langle x|\mathrm{d}x\right) |\psi\rangle \tag{156}$$

[1 mark] and

$$\begin{aligned} 1 &= \langle\psi|\hat{\mathbb{I}}|\psi\rangle \\ &= \langle\psi|\psi\rangle \end{aligned}$$

[1 mark].

(iii)

$$\int_{-\infty}^{\infty} \varphi(x)^* \left(\hat{A}\psi(x)\right) \mathrm{d}x = \int_{-\infty}^{\infty} \left(\hat{A}\varphi(x)\right)^* \psi(x)\,\mathrm{d}x \tag{157}$$

[1 mark]

where $\varphi(x)$, $\psi(x)$ are normalisable, requiring them to vanish at $x = \pm\infty$ **[1 mark]**.

(iv) (a) Hermitian – it's observable (the position). You can also check explicitly using the equation just stated.

(b) Hermitian – it's observable (the momentum). You can also check explicitly using the equation just stated.

(c) Not hermitian. To see this, note that the previous result was Hermitian, meaning

$$(-i\hbar\partial_x)^\dagger = -i\hbar\partial_x \tag{158}$$

and therefore for that to be true it must be the case that

$$(\partial_x)^\dagger = -\partial_x. \tag{159}$$

Explicitly we can use the expression for the Hermitian conjugate:

$$\int_{-\infty}^{\infty} \varphi(x)^* (\partial_x \psi(x))\, \mathrm{d}x = -\int_{-\infty}^{\infty} \partial_x \left(\varphi(x)^*\right) \psi(x)\, \mathrm{d}x \tag{160}$$

$$= \int_{-\infty}^{\infty} \left(-\partial_x \varphi(x)^*\right) \psi(x)\, \mathrm{d}x \tag{161}$$

where the first line uses integration by parts and the fact that the wavefunctions must vanish at infinity for them to be normalisable (so there is no boundary term in the integration by parts).

(d) Hermitian, because $\hat{p}^2$ is Hermitian (as it's a power of a Hermitian operator) and so

$$\left((-i\hbar\partial_x)^2\right)^\dagger = (-i\hbar\partial_x)^2 \tag{162}$$

and

$$\left(\partial_x^2\right)^\dagger = \partial_x^2. \tag{163}$$

Alternatively, use (c) and square both sides.

(e) Not Hermitian. As in (c), $\nabla^\dagger = -\nabla$.

(v) This question is not something which has been seen in the lectures or notes, but the maths isn't too hard.

Insert two copies of the identity:

$$\langle\psi|\hat{A}|\psi\rangle = \langle\psi|\hat{\mathbb{I}}|\hat{A}|\hat{\mathbb{I}}|\psi\rangle \tag{164}$$

[1 mark]

$$\langle\psi|\hat{A}|\psi\rangle = \langle\psi|\int_{-\infty}^{\infty}|x\rangle\langle x|\mathrm{d}x|\hat{A}|\int_{-\infty}^{\infty}|y\rangle\langle y|\mathrm{d}y|\psi\rangle \tag{165}$$

[1 mark] where we have used different position labels to avoid confusion. Since $|\psi\rangle$ is not a function of position, we can pull the integrals outside:

$$\begin{aligned}\langle\psi|\hat{A}|\psi\rangle &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\langle\psi|x\rangle\langle x|\hat{A}|y\rangle\langle y|\psi\rangle\mathrm{d}x\mathrm{d}y && (166)\\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi^{*}(x)\,\langle x|\hat{A}|y\rangle\psi(y)\,\mathrm{d}x\mathrm{d}y && (167)\end{aligned}$$

[1 mark] to give the desired result

$$\langle\psi|\hat{A}|\psi\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi^{*}(x)\,A(x,y)\,\psi(y)\,\mathrm{d}x\mathrm{d}y \tag{168}$$

provided that

$$A(x,y) = \langle x|\hat{A}|y\rangle. \tag{169}$$

[1 mark].

(vi) This is a tricky question to differentiate the top students. It is not relied upon in the last part of the question, which helps justify its presence here. The answer is that physical operators act *locally*: they act at a point in space, not across all of space simultaneously **[1 mark]**. We can deduce the properties of a particle by measuring the particle at a given location. Therefore an operator cannot really be an independent function of two separate position co-ordinates, as that would mean it depended not only on what is happening *here*, but also *there*, for all possible *theres*. And that would be very strange.

The Dirac delta function encodes this, as it is zero unless $x = y$ **[1 mark]**.

(vii) Using the expression provided in the previous part,

$$\langle\psi|\hat{A}|\psi\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi^*(x)\, A(x)\, \delta(x-y)\, \psi(y)\, \mathrm{d}x\mathrm{d}y \tag{170}$$

[1 mark]

and use the definition of the Dirac delta function

$$\int_{-\infty}^{\infty} f(x)\, \delta(x-y)\, \mathrm{d}x = f(y) \tag{171}$$

[1 mark]

to give

$$\langle\psi|\hat{A}|\psi\rangle = \int_{-\infty}^{\infty} \psi^*(x)\, A(x)\, \psi(x)\, \mathrm{d}x. \tag{172}$$

7.2 Question

(i) It is an axiom of quantum mechanics that states of a system are represented by normalized kets $|\psi\rangle$ in a complex Hilbert space $\mathcal{H}$. Explain physically why the states must be normalized, and give an expression for this mathematically.

[2 marks]

(ii) Write the normalization condition for a wavefunction $\psi(x)$ written in the position basis.

[1 mark]

(iii) Below are the ten axioms defining a linear vector space for vectors $|u\rangle$ (written formally, but with translations into English where unclear). Show that each axiom is obeyed by complex functions $f(x)$.
$\forall \{|u\rangle, |v\rangle, |w\rangle\} \in V;\ \alpha, \beta \in \mathbb{C}:$
[for all vectors $|u\rangle, |v\rangle, |w\rangle$ in the linear vector space V, with α and β complex numbers]
1. $|u\rangle + |v\rangle \in V$ [If $|u\rangle$ and $|v\rangle$ are in the vector space, then so is $|u\rangle + |v\rangle$]
2. $(|u\rangle + |v\rangle) + |w\rangle = |u\rangle + (|v\rangle + |w\rangle)$ [associativity]
3. $\exists |0\rangle \in V:\ |u\rangle + |0\rangle = |0\rangle + |u\rangle = |u\rangle$ [there exists a zero vector $|0\rangle$ such that adding this to any vector leaves that vector unchanged]
4. $\exists (-|u\rangle) \in V:\ |u\rangle + (-|u\rangle) = |0\rangle$ [for all vectors in the space there exists an additive inverse which, when added to the vector, gives the zero vector]
5. $|u\rangle + |v\rangle = |v\rangle + |u\rangle$ [commutativity]
6. $\alpha|u\rangle \in V$ [α times a vector in V is also in V]
7. $\alpha(|u\rangle + |v\rangle) = \alpha|u\rangle + \alpha|v\rangle$ [distributivity]
8. $(\alpha + \beta)|u\rangle = \alpha|u\rangle + \beta|u\rangle$
9. $\alpha(\beta|u\rangle) = (\alpha\beta)|u\rangle$
10. $1|u\rangle = |u\rangle$.

[3 marks]

(iv) Using the fact that $\langle x|\psi\rangle = \psi(x)$, and (i) and (ii), deduce the *resolution of the identity*

$$\hat{\mathbb{I}} = \int_{-\infty}^{\infty} |x\rangle\langle x| \mathrm{d}x. \tag{173}$$

[3 marks]

(v) Hence show that

$$\langle f|g\rangle \triangleq \int_{-\infty}^{\infty} f(x)^* g(x)\, \mathrm{d}x. \tag{174}$$

[2 marks]

(vi) Below are the three axioms defining an inner product space. For each, show that it is obeyed by complex functions.

1. $\langle u|v\rangle = (\langle v|u\rangle)^*$
2. $\langle u|u\rangle \geq 0$; $\langle u|u\rangle = 0$ iff $|u\rangle = |0\rangle$
3. $\langle w|\,(\alpha|u\rangle + \beta|v\rangle) = \alpha\langle w|u\rangle + \beta\langle w|v\rangle$.

[3 marks]

(vii) In quantum mechanics observable quantities are represented by Hermitian operators $\hat{A}$. It is assumed these possess a complete set of orthogonal eigenstates $|a_n\rangle$:

$$\hat{A}|a_n\rangle = a_n|a_n\rangle. \tag{175}$$

State the possible results of a measurement of the observable $\hat{A}$, and the probabilities to find each outcome.

[2 marks]

(viii) The position of a particle is an observable quantity. Assuming there is a discrete set of possible positions, state the equivalent form of Eq 175 for position, explaining the meaning of any terms.

[2 marks]

(ix) By reference to your answer to (vii), state the possible results of a measurement of position, and the probabilities to find each outcome. Explain any subtleties which arise when space becomes continuous.

[2 marks]

8 The quantum harmonic oscillator

Please hand in answers via turnitin no later than **2pm Monday week 8 (21st November)**.

8.0 Videos

Please watch videos: **V8.1, V8.2, V8.3, V8.4**.

8.1 Worked Example

(i) The Hamiltonian for the quantum harmonic oscillator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2. \tag{176}$$

Write the corresponding TISE in the position basis, denoting the n^{th} energy eigenstate $\phi_n(x)$ and the corresponding energy eigenvalue E_n.

[2 marks, A]

(ii) Defining the lowering operator

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{\hbar}{m\omega}\partial_x\right) \tag{177}$$

and the raising operator

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{\hbar}{m\omega}\partial_x\right) \tag{178}$$

Show that the TISE can be rewritten as

$$\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\phi_n(x) = E_n\phi_n(x). \tag{179}$$

[4 marks, C]

(iii) Show that

$$\left[\hat{a}, \hat{a}^\dagger\right] f(x) = f(x) \tag{180}$$

for any function $f(x)$.

[3 marks, C]

(iv) Hence, by acting on both sides of the TISE with $\hat{a}^\dagger$,show that

$$\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\left(\hat{a}^\dagger\phi_n(x)\right) = \left(E_n + \hbar\omega\right)\left(\hat{a}^\dagger\phi_n(x)\right). \tag{181}$$

[3 marks, C]

(v) Solve

$$\hat{a}\phi_0(x) = 0. \tag{182}$$

[3 marks, C]

(vi) Explain what (iv) and (v) tell us about the energy eigenvalues of the harmonic oscillator.

[2 marks, C]

(vii) Without worrying about normalization, calculate $\phi_1(x)$ and $\phi_2(x)$ and sketch the results.

[3 marks, E]

Answers to 8.1

(i)

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi_n(x)}{\partial x^2}+\frac{1}{2}m\omega^2x^2\phi_n(x)=E_n\phi_n(x). \tag{183}$$

[1 mark] for writing out operators in the position basis correctly.

[1 mark] for getting the right answer.

(ii) It's probably easiest to work backwards.

$$\hbar\omega\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)\phi_n(x)=\hbar\omega\left(\frac{m\omega}{2\hbar}\left(x-\frac{\hbar}{m\omega}\partial_x\right)\left(x+\frac{\hbar}{m\omega}\partial_x\right)+\frac{1}{2}\right)\phi_n(x) \tag{184}$$

$$=\frac{m\omega^2}{2}\left(x-\frac{\hbar}{m\omega}\partial_x\right)\left(x+\frac{\hbar}{m\omega}\partial_x\right)\phi_n(x)+\frac{\hbar\omega}{2}\phi_n(x) \tag{185}$$

[1 mark]

$$=\frac{m\omega^2}{2}\left(x^2\phi_n(x)-\left(\frac{\hbar}{m\omega}\right)^2\partial_x^2\phi_n(x)+x\frac{\hbar}{m\omega}\partial_x\phi_n(x)-\frac{\hbar}{m\omega}\partial_x\left(x\phi_n(x)\right)\right)+\frac{\hbar\omega}{2}\phi_n(x) \tag{186}$$

[1 mark]

$$=\frac{m\omega^2}{2}\left(x^2\phi_n(x)-\left(\frac{\hbar}{m\omega}\right)^2\partial_x^2\phi_n(x)+\cancel{x\frac{\hbar}{m\omega}\partial_x\phi_n(x)}-\cancel{\frac{\hbar}{m\omega}\phi_n(x)}-\cancel{\frac{\hbar}{m\omega}x\partial_x\phi_n(x)}\right)+\cancel{\frac{\hbar\omega}{2}\phi_n(x)} \tag{187}$$

where strikethroughs match in pairs of the same angle **[1 mark]**.

This gives

$$\hbar\omega\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)\phi_n(x)=-\frac{\hbar^2}{2m}\partial_x^2\phi_n(x)+\frac{1}{2}m\omega^2x^2\phi_n(x) \tag{188}$$

as required **[1 mark]**.

(iii)

$$\begin{aligned}\left[\hat{a},\hat{a}^\dagger\right]f&=\hat{a}\hat{a}^\dagger f-\hat{a}^\dagger\hat{a}f\\&=\frac{m\omega}{2\hbar}\left(x+\frac{\hbar}{m\omega}\partial_x\right)\left(x-\frac{\hbar}{m\omega}\partial_x\right)f-\frac{m\omega}{2\hbar}\left(x-\frac{\hbar}{m\omega}\partial_x\right)\left(x+\frac{\hbar}{m\omega}\partial_x\right)f\end{aligned}$$

[1 mark]

$$
\begin{aligned}
&= \frac{m\omega}{2\hbar}\left(x^2 f - \left(\frac{\hbar}{m\omega}\right)^2 \partial_x^2 f - x\frac{\hbar}{m\omega}\partial_x f + \frac{\hbar}{m\omega}\partial_x (xf)\right) \\
&- \frac{m\omega}{2\hbar}\left(x^2 f - \left(\frac{\hbar}{m\omega}\right)^2 \partial_x^2 f + x\frac{\hbar}{m\omega}\partial_x f - \frac{\hbar}{m\omega}\partial_x (xf)\right) \\
&= -x\partial_x f + \partial_x (xf) \\
&= -x\partial_x f + f + x\partial_x f \\
&= f
\end{aligned}
$$

[2 marks] for reasonable working.

(iv) It's much easier to work with

$$\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\phi_n(x) = E_n\phi_n(x)\,. \tag{189}$$

Then we have

$$\hbar\omega\left(\hat{a}^\dagger\hat{a}^\dagger\hat{a}\phi_n(x) + \frac{1}{2}\hat{a}^\dagger\phi_n(x)\right) = E_n\hat{a}^\dagger\phi_n(x) \tag{190}$$

[1 mark]. Use the commutation relation just found:

$$\hat{a}^\dagger\hat{a}\phi_n(x) = \hat{a}\hat{a}^\dagger\phi_n(x) - \phi_n(x) \tag{191}$$

[1 mark] to give

$$\hbar\omega\left(\hat{a}^\dagger\hat{a}\hat{a}^\dagger\phi_n(x) - \hat{a}^\dagger\phi_n(x) + \frac{1}{2}\hat{a}^\dagger\phi_n(x)\right) = E_n\hat{a}^\dagger\phi_n(x) \tag{192}$$

[1 mark]. Therefore

$$\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\left(\hat{a}^\dagger\phi_n(x)\right) = (E_n + \hbar\omega)\left(\hat{a}^\dagger\phi_n(x)\right) \tag{193}$$

as required.

(v)

$$\hat{a}\phi_0(x) = 0 \tag{194}$$

$$\left(x + \frac{\hbar}{m\omega}\partial_x\right)\phi_0(x) = 0 \tag{195}$$

$$x\phi_0(x) + \frac{\hbar}{m\omega}\frac{\partial\phi_0(x)}{\partial x} = 0 \tag{196}$$

$$x\phi_0(x) + \frac{\hbar}{m\omega}\frac{\mathrm{d}\phi_0(x)}{\mathrm{d}x} = 0 \tag{197}$$

[1 mark] for realising that the partial derivative becomes a total derivative (the key step).

$$\int \frac{\mathrm{d}\phi_0(x)}{\phi_0(x)} = -\frac{m\omega}{\hbar}\int x\mathrm{d}x \tag{198}$$

[1 mark] giving

$$\ln(\phi_0(x)) = -\frac{m\omega}{2\hbar}x^2 + C \tag{199}$$

and

$$\phi_0(x) = A\exp\left(-\frac{m\omega}{2\hbar}x^2\right) \tag{200}$$

[1 mark]. There is no need to normalise.

(vi)

Part (iv) tells us that there is an infinite ladder of energies separated by $\hbar\omega$ **[1 mark]**.

Part (v) tells us that there is a lowest rung to the ladder, i.e. a ground state **[1 mark]**.

(vii) This requires us to recall that

$$\hat{a}^\dagger\phi_0(x) \propto \phi_1(x) \tag{201}$$

$$\left(\hat{a}^\dagger\right)^2\phi_0(x) \propto \phi_2(x) \tag{202}$$

[1 mark]. Therefore

$$\phi_1(x) \propto \left(x - \frac{\hbar}{m\omega}\partial_x\right)\exp\left(-\frac{m\omega}{2\hbar}x^2\right) \tag{203}$$

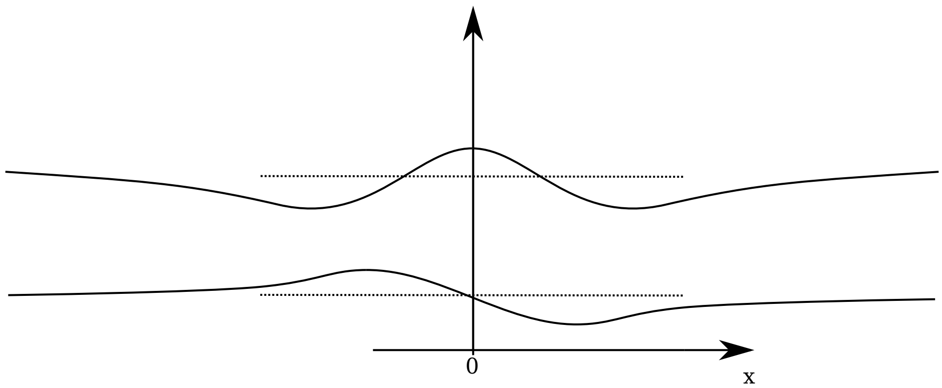
$$= 2x\exp\left(-\frac{m\omega}{2\hbar}x^2\right) \tag{204}$$

and

$$\phi_2(x) \propto \left(x - \frac{\hbar}{m\omega}\partial_x\right)\left(x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\right) \tag{205}$$
$$= x^2\exp\left(-\frac{m\omega}{2\hbar}x^2\right) - \frac{\hbar}{m\omega}\exp\left(-\frac{m\omega}{2\hbar}x^2\right) + x^2\exp\left(-\frac{m\omega}{2\hbar}x^2\right) \tag{206}$$
$$= \left(2x^2 - \frac{\hbar}{m\omega}\right)\exp\left(-\frac{m\omega}{2\hbar}x^2\right) \tag{207}$$

[1 mark].

Sketches for **[1 mark]** total:



(no need to offset vertically; can be plotted on different axes).

8.2 Question

(i) The Hamiltonian for the quantum harmonic oscillator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2. \tag{208}$$

Write the corresponding TISE in a basis independent way, denoting the n^{th} energy eigenstate $|n\rangle$ and the corresponding energy eigenvalue E_n.

[2 marks]

(ii) Defining the lowering operator

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) \tag{209}$$

and the raising operator

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right) \tag{210}$$

Show that the Hamiltonian can be rewritten as

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\hat{\mathbb{I}}\right). \tag{211}$$

[4 marks]

(iii) Using the canonical commutation relation, show that

$$\left[\hat{a}, \hat{a}^\dagger\right] = \hat{\mathbb{I}}. \tag{212}$$

[3 marks]

(iv) Hence, by acting on both sides of the TISE with $\hat{a}^\dagger$,show that

$$\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\hat{\mathbb{I}}\right)\left(\hat{a}^\dagger|n\rangle\right) = \left(E_n + \hbar\omega\right)\left(\hat{a}^\dagger|n\rangle\right). \tag{213}$$

[3 marks]

(v) Hence explain why $\hat{a}^\dagger$ is called the raising operator.

[2 marks]

(vi) Explain why $|n\rangle$ must be an eigenstate of $\hat{a}^\dagger\hat{a}$.

[2 marks]

(vii) The corresponding eigenvalues are

$$\hat{a}^\dagger\hat{a}|n\rangle = n|n\rangle. \tag{214}$$

Find a lower bound on the ground state energy of the quantum harmonic oscillator.

[4 marks]

9 The Schrödinger equation in three dimensions

Please hand in answers via turnitin no later than **2pm Monday week 9 (30th November)**.

9.0 Videos

Please watch videos: **V9.1, V9.2, V9.3, V9.4**.

9.1 Worked Example

The three-dimensional infinite-potential (cubic) well is defined by the potential

$$V(\boldsymbol{r}) = \begin{cases} 0, & 0 \leq r_i \leq L \\ \infty, & \text{otherwise} \end{cases} \tag{215}$$

where $\boldsymbol{r} = (x, y, z)$ and r_i is element i of $\boldsymbol{r}$.

(i) Sketch the potential.

[2 marks, C]

(ii) Write down the time-independent Schrödinger equation for this potential, explaining any terms you introduce.

[1 mark, A]

(iii) Using separation of variables, show that this reduces to three independent copies of the TISE for the 1D infinite potential well.

[5 marks, C]

(iv) The energies are therefore given by

$$E_{\boldsymbol{n}} = \frac{\hbar^2 \pi^2}{2mL^2} \left(n_x^2 + n_y^2 + n_z^2\right) \tag{216}$$

with n_i integers greater than zero. Find the degeneracy of the lowest four energy levels of the 3D infinite potential well.

[4 marks, E]

(v) The 3D angular momentum operators $\hat{L}_i$, where $i \in [x, y, z]$, obey the commutation relation

$$\left[\hat{L}_i, \hat{L}_j\right] = i\hbar\epsilon_{ijk} L_k \tag{217}$$

where ϵ_{ijk} is the Levi-Civita symbol, which is +1 for $ijk = xyz$ and cyclic permutations, −1 for $ijk = zxy$ and cyclic permutations, and 0 otherwise.

Defining

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y \tag{218}$$

show that

$$\left[\hat{L}_\pm, \hat{L}_z\right] = \mp\hbar\hat{L}_\pm. \tag{219}$$

(Recall that the ± symbol indicates two separate equations, one for the top symbol and one for the bottom.)

[3 marks, C]

(vi) Show that

$$\left[\hat{L}^2, \hat{L}_z\right] = 0. \tag{220}$$

[Hint]: you may need to use the fact that

$$\left[A^2, B\right] = A\left[A, B\right] + \left[A, B\right]A. \tag{221}$$

[3 marks, C]

(vii) Explain what the result of (vi) means in terms of what can be known about the angular momentum.

[2 marks, F]

Answers to 9.1

(i) [a cubic box with $V = 0$ inside, and $V = \infty$ outside.] [1 mark] for a cube with the right potentials indicated, [1 mark] for the correct axis labels.

(ii)

$$-\frac{\hbar^2}{2m}\nabla^2\Phi_{\boldsymbol{n}}(\boldsymbol{r}) = E_{\boldsymbol{n}}\Phi_{\boldsymbol{n}}(\boldsymbol{r}) \tag{222}$$

where $\boldsymbol{n} = (n_x, n_y, n_z)$ is a set of integers with $n_i > 0$, and $\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$.

(iii)

Try the ansatz

$$\Phi_{\boldsymbol{n}}(\boldsymbol{r}) = \phi^x_{n_x}(x)\,\phi^y_{n_y}(y)\,\phi^z_{n_z}(z) \tag{223}$$

with

$$E_{\boldsymbol{n}} \triangleq E_{n_x} + E_{n_y} + E_{n_z} \tag{224}$$

[1 mark]. This gives

$$\frac{\hbar^2}{2m}\left(\partial_x^2 + \partial_y^2 + \partial_z^2\right)\phi^x_{n_x}(x)\,\phi^y_{n_y}(y)\,\phi^z_{n_z}(z) = \left(E_{n_x} + E_{n_y} + E_{n_z}\right)\phi^x_{n_x}(x)\,\phi^y_{n_y}(y)\,\phi^z_{n_z}(z) \tag{225}$$

[1 mark] and

$$\frac{\hbar^2}{2m}\left(\phi^y_{n_y}(y)\,\phi^z_{n_z}(z)\,\partial_x^2\phi^x_{n_x}(x) + c.p.\right) = \left(E_{n_x} + E_{n_y} + E_{n_z}\right)\phi^x_{n_x}(x)\,\phi^y_{n_y}(y)\,\phi^z_{n_z}(z) \tag{226}$$

$$\frac{\hbar^2}{2m}\left(\phi^y_{n_y}(y)\,\phi^z_{n_z}(z)\,\frac{\mathrm{d}^2\phi^x_{n_x}(x)}{\mathrm{d}x^2} + c.p.\right) = \left(E_{n_x} + E_{n_y} + E_{n_z}\right)\phi^x_{n_x}(x)\,\phi^y_{n_y}(y)\,\phi^z_{n_z}(z) \tag{227}$$

where c.p. indicates all cyclic permutations of x, y, z. The partial derivative becomes a total derivative as it acts on a function which depends on no other variables **[1 mark]**. This is the key to the separation of variables method.

Now divide through by $\Phi_{\boldsymbol{n}}(\boldsymbol{x})$:

$$\frac{\hbar^2}{2m}\left(\left(\phi^x_{n_x}\right)^{-1}\mathrm{d}_x^2\phi^x_{n_x}(x) + \left(\phi^y_{n_y}\right)^{-1}\mathrm{d}_y^2\phi^y_{n_y}(y) + \left(\phi^z_{n_z}\right)^{-1}\mathrm{d}_z^2\phi^z_{n_z}(z)\right) = E_{n_x} + E_{n_y} + E_{n_z} \tag{228}$$

[1 mark]. Finally, note that

$$\left(\frac{\hbar^2}{2m}\left(\phi^x_{n_x}\right)^{-1}\mathrm{d}^2_x\phi^x_{n_x}(x) - E_{n_x}\right) + (x \to y) + (x \to z) = 0. \tag{229}$$

Therefore a solution is provided if $\phi^x_{n_x}$ solves

$$\frac{\hbar^2}{2m}\partial^2_x\phi^x_{n_x}(x) = E_{n_x}\phi^x_{n_x}(x) \tag{230}$$

and similarly for $\phi^y_{n_y}$ and $\phi^z_{n_z}$ **[1 mark]**.
This is nothing other than three independent copies of the 1D TISE for the infinite potential well, as required.
(iv) The easiest way to do this is to tabulate the energies.

(n_x, n_y, n_z)	$E_{\boldsymbol{n}} \cdot 2mL^2/\left(\hbar^2\pi^2\right)$	degeneracy
$(1,1,1)$	3	1
$(1,1,2)$	6	3
$(1,2,2)$	9	3
$(1,1,3)$	11	3
$(2,2,2)$	12	1

[1 mark] for each of the first 4 rows; the 5th is just there because I had to check which of the last two was lower in energy (may as well leave it there in case of error!). The degeneracy is found in each case by working out the possible re-arrangements of the numbers in the first column which would give the same number in the second column.
(v)

$$\left[\hat{L}_\pm, \hat{L}_z\right] = \left[\hat{L}_x \pm i\hat{L}_y, \hat{L}_z\right] \tag{231}$$
$$= \left[\hat{L}_x, \hat{L}_z\right] \pm i\left[\hat{L}_y, \hat{L}_z\right] \tag{232}$$
$$= -i\hbar\hat{L}_y \pm i\left(i\hbar\hat{L}_x\right) \tag{233}$$
$$= \mp\hbar\left(\hat{L}_x \pm i\hat{L}_y\right) \tag{234}$$
$$= \mp\hbar\hat{L}_\pm. \tag{235}$$

[1 mark] for lines 1, 3, 4.
(vi)

$$\left[\hat{L}^2, \hat{L}_z\right] = \left[\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_z\right] \tag{236}$$
$$= \left[\hat{L}_x^2 + \hat{L}_y^2, \hat{L}_z\right] \tag{237}$$
$$= \left[\hat{L}_x^2, \hat{L}_z\right] + \left[\hat{L}_y^2, \hat{L}_z\right] \tag{238}$$

[1 mark]. Using the relation provided,

$$\left[\hat{L}^2, \hat{L}_z\right] = \hat{L}_x\left[\hat{L}_x, \hat{L}_z\right] + \left[\hat{L}_x, \hat{L}_z\right]\hat{L}_x + \hat{L}_y\left[\hat{L}_y, \hat{L}_z\right] + \left[\hat{L}_y, \hat{L}_z\right]\hat{L}_y \tag{239}$$
$$= -i\hbar\hat{L}_x\hat{L}_y - i\hbar\hat{L}_y\hat{L}_x + i\hbar\hat{L}_y\hat{L}_x + i\hbar\hat{L}_x\hat{L}_y \tag{240}$$
$$= 0 \tag{241}$$

[1 mark] for each of the first 2 lines.

(vii) Since the operators commute, we can have simultaneous knowledge of the corresponding observables **[1 mark]**.

In this case, the corresponding observables are the square of the total angular momentum, and the $z-$projection of the angular momentum. **[1 mark]**.

9.2 Question

The three-dimensional harmonic oscillator is defined by the potential

$$V(\boldsymbol{r}) = \frac{1}{2}m\omega^2\boldsymbol{r}^2 \tag{242}$$

where $\boldsymbol{r} = (x, y, z)$.

(i) Write down the time-independent Schrödinger equation for this potential, explaining any terms you introduce.

[1 mark]

(ii) Using separation of variables, show that this reduces to three independent copies of the TISE for the 1D harmonic oscillator.

[5 marks]

(iii) The energies are therefore given by

$$E_{\boldsymbol{n}} = \hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right) \tag{243}$$

with n_i integers greater than or equal to zero. Find the degeneracy of the lowest four energy levels of the 3D harmonic oscillator.

[4 marks]

(iv) What would be the degeneracy of the lowest *three* energy levels if the potential were instead

$$V(\boldsymbol{r}) = \frac{1}{2}m\omega_1^2x^2 + \frac{1}{2}m\omega_1^2y^2 + \frac{1}{2}m\omega_2^2z^2 \tag{244}$$

with $\omega_2 > \omega_1$?

[4 marks]

(v) Denote the eigenstates of the operator $\hat{L}_z$, which represents the $z-$projection of the angular momentum,

$$\hat{L}_z|m\rangle = \hbar m|m\rangle. \tag{245}$$

The operators $\hat{L}_\pm$ obey the commutation relation

$$\left[\hat{L}_\pm, \hat{L}_z\right] = \mp\hbar\hat{L}_\pm. \tag{246}$$

By showing the effect of $\hat{L}_\pm$ on $|m\rangle$, explain why $\hat{L}_\pm$ are called ladder operators.

[6 marks]

10 The Hydrogen Atom

Please hand in answers via turnitin no later than **2pm Monday week 10 (7th December)**.

10.0 Videos

Please watch videos: **V10.1**, **V10.2**, **V10.3.**

10.1 Worked example

(i) State the assumptions going into Bohr's (incorrect) model of the electronic states in the atom.

[3 marks, A]

(ii) Write a mathematical expression encoding Bohr's statement regarding the quantization of angular momentum.

[2 marks, A]

(iii) The energy levels of the atom in the Bohr model are:

$$E_n = \frac{m_e e^4}{2\left(4\pi\epsilon_0\right)^2 \hbar^2 n^2}. \tag{247}$$

Use this formula to calculate the ionization energy of hydrogen.

[3 marks, C]

(iv) What would be the equivalent formula for positronium (an electron-positron bound state)?

[1 mark, G]

(v) A more accurate model is provided by quantum mechanics. For a particle of mass m_e, in polar co-ordinates

$$\boldsymbol{r} = (r, \theta, \phi) \tag{248}$$

the TISE reads

$$\left(-\frac{\hbar^2}{2\mathrm{m}_e r^2}\partial_r\left(r^2\partial_r\right) - \frac{\hbar^2}{2\mathrm{m}_e r^2}\left(\frac{1}{\sin(\theta)}\partial_\theta\left(\sin(\theta)\,\partial_\theta\right) + \frac{1}{\sin^2(\theta)}\partial_\phi^2\right) + V(\boldsymbol{r})\right)\psi(\boldsymbol{r},t) = E\psi(\boldsymbol{r},t). \tag{249}$$

State the condition on $V(\boldsymbol{r})$ for it to be spherically symmetrical.

[1 mark, A]

(vi) Explain why, if the potential is spherically symmetrical, the TISE is separable using the ansatz

$$\psi(\boldsymbol{r},t) = T(t)\,R(r)\,Y(\theta,\phi). \tag{250}$$

[2 marks, C]

(vii) Carry out the separation into two ODEs, the radial and angular equations. Setting each equal to the same constant $\hbar^2 k^2$ you should find the radial equation

$$\hbar^2 \frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \frac{\mathrm{d}}{\mathrm{d}r}\right) R + 2mr^2 \left(E - V\right) R = \hbar^2 k^2 R$$

and angular equation

$$\hat{L}^2 Y = \hbar^2 k^2 Y.$$

[4 marks, D]

(viii) Explain why the TISE of the electron in the hydrogen atom takes the form

$$\left(-\frac{\hbar^2}{2\mu r^2}\partial_r\left(r^2\partial_r\right) + \frac{\hbar^2 l\left(l+1\right)}{2\mu r^2} - \frac{e^2}{4\pi\epsilon_0 r}\right)\varphi_{n,l,m}\left(\boldsymbol{r}\right) = E_n \varphi_{n,l,m}\left(\boldsymbol{r}\right) \qquad (251)$$

explaining the meaning of μ.

[4 marks, D]

Answers to 10.1

(i)

- Electrons travel along circular orbits **[1 mark]**.
- The angular momentum of the electron along these orbits is an integer multiple of $\hbar$ **[1 mark]**.
- The electron can only gain or lose energy via transitions from one orbit to another **[1 mark]**.

(ii)

$$L = mvr = n\hbar \tag{252}$$

[1 mark] where m is the mass of the electron, v is its velocity, r is the radius of the orbit, n is an integer and $\hbar$ is Planck's constant **[1 mark]**.

(iii)

The ionization energy is the energy to excite the electron from state $n = 1$ to $n = \infty$ (unbound) **[1 mark]**.

Therefore

$$\begin{aligned} E_{\text{ionization}} &= \frac{m_e e^4}{2\left(4\pi\epsilon_0\right)^2 \hbar^2} \, [1\,\text{mark}] \\ &= 13.6\,\text{eV}. \, [1\,\text{mark}] \end{aligned}$$

(iii)

In this case use the reduced mass $\mu = \left(m_e^{-1} + m_p^{-1}\right)^{-1} \approx m_e/2$ to give

$$E_n^{\text{positronium}} = \frac{1}{2} E_n^H. \, [1\,\text{mark}]$$

We should really have used the reduced mass in the hydrogen case as well, but for hydrogen the difference from the electron mass is smaller than the stated precision.

(iv)

$V(\boldsymbol{r}) = V(r)$.

(v)

in the case that $V = V(r)$ the Hamiltonian is just a sum of operators acting on either r or (θ, ϕ). **[1 mark]**

This is a sufficient condition for separability. **[1 mark]**

(Or the student may show the result explicitly by beginning the separation process.)

(vi)

Substitute the ansatz:

$$\left(-\frac{\hbar^2}{2mr^2}\partial_r\left(r^2\partial_r\right)+V\left(r\right)\right)R\left(r\right)Y\left(\theta,\phi\right)+\frac{1}{2mr^2}\hat{L}^2R\left(r\right)Y\left(\theta,\phi\right)=ER\left(r\right)Y\left(\theta,\phi\right) \tag{253}$$

$$\downarrow$$

$$\hat{L}^2R\left(r\right)Y\left(\theta,\phi\right)=\left(\hbar^2\partial_r\left(r^2\partial_r\right)+2mr^2\left(E-V\left(r\right)\right)\right)R\left(r\right)Y\left(\theta,\phi\right) \tag{254}$$

$$\downarrow \text{divide by } \psi$$

$$\frac{1}{Y}\hat{L}^2Y\left(\theta,\phi\right)=\frac{1}{R}\hbar^2\partial_r\left(r^2\partial_r\right)R\left(r\right)+2mr^2\left(E-V\left(r\right)\right). \tag{255}$$

Since both sides are always equal, while the left is a function only of r and the right is a function only of θ and ϕ, they must both equal the same constant. Call this $\hbar^2k^2$ as requested:

$$\frac{1}{R}\hbar^2\partial_r\left(r^2\partial_r\right)R+\frac{2mr^2}{R}\left(E-V\right)R\triangleq\hbar^2k^2\,[1\,mark] \tag{256}$$

$$\frac{1}{Y}\hat{L}^2Y\triangleq\hbar^2k^2\,[1\,mark]. \tag{257}$$

Finally, multiply the top equation through by R, noting that the resulting radial equation is now an ODE:

$$\hbar^2\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}}{\mathrm{d}r}\right)R+2mr^2\left(E-V\right)R=\hbar^2k^2R\,[1\,mark].$$

And multiply the bottom equation by Y giving the angular equation, which at this stage is still a PDE:

$$\hat{L}^2Y=\hbar^2k^2Y.\,[1\,mark]$$

(vii)

Since

$$\hat{L}^2|l\rangle=\hbar^2l\left(l+1\right)|l\rangle$$

the eigenstates of the angular equation are

$$\hat{L}^2|l\rangle = \hbar^2 l\,(l+1)\,|l\rangle = \hbar^2 k^2 |l\rangle$$

so $k^2 = l\,(l+1)$. **[1 mark]**

Substituting the same result into the radial equation gives

$$\hbar^2 \frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \frac{\mathrm{d}}{\mathrm{d}r}\right) R_l + 2mr^2\,(E-V)\,R_l = \hbar^2 l\,(l+1)\,R_l \;[1\,\mathrm{mark}]$$

where $R\,(r)$ is now labelled by l, as this appears in its defining equation here.

(viii)

The Coulomb potential energy of the electron in the presence of the nucleus is

$$V\,(\boldsymbol{r}) = -\frac{e^2}{4\pi\epsilon_0 r}$$

[1 mark]. This is spherically symmetrical **[1 mark]**. The labels n, l, and m are all good quantum numbers **[1 mark]**; μ is the reduced mass of the electron **[1 mark].**

10.2 Question

(i) State the assumptions going into Bohr's (incorrect) model of the electronic states in the atom.

[3 marks]

(ii) Write a mathematical expression encoding Bohr's statement regarding the quantization of angular momentum.

[2 marks]

(iii) Assuming (incorrectly) that the electron orbits the nucleus classically, equate the centripetal force to the electrostatic force to obtain an expression for the electron's velocity in terms of the radius of its orbit.

[3 marks]

(iv) Hence, using (ii) and (iii), derive Bohr's formula for the kinetic energy of the electron in the n^{th} orbit

$$E_n = \frac{m_e e^4}{2\left(4\pi\epsilon_0\right)^2 \hbar^2 n^2}. \tag{258}$$

[3 marks]

(v) A more accurate model is provided by quantum mechanics. The TISE describing an electron in the electrostatic potential of a proton is

$$\left(-\frac{\hbar^2}{2\mu r^2}\partial_r\left(r^2\partial_r\right) + \frac{\hbar^2 l\left(l+1\right)}{2\mu r^2} - \frac{e^2}{4\pi\epsilon_0 r}\right)\varphi_{n,l,m}\left(\boldsymbol{r}\right) = E_n\varphi_{n,l,m}\left(\boldsymbol{r}\right) \tag{259}$$

where $\boldsymbol{r} = (r,\theta,\phi)$ is the position in spherical polar co-ordinates, μ is the reduced mass of the electron, e is the charge of the electron, ϵ_0 is the permittivity of free space, and $\hbar$ is the reduced Planck's constant. Explain the meaning of the quantum numbers n, l, and m.

[3 marks]

(vi) Using the ansatz

$$\varphi_{n,l,m}\left(\boldsymbol{r}\right) = \frac{\chi_{n,l}\left(r\right)}{r}Y_l^m\left(\theta,\phi\right) \tag{260}$$

show that $\chi_{n,l}\left(r\right)$ solves the radial equation

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2\chi_{n,l}\left(r\right)}{\mathrm{d}r^2} - \frac{e^2}{4\pi\epsilon_0 r}\chi_{n,l}\left(r\right) + \frac{\hbar^2 l\left(l+1\right)}{2\mu r^2}\chi_{n,l}\left(r\right) = E_n\chi_{n,l}\left(r\right). \tag{261}$$

[4 marks]

(vii) Find an approximate solution in the limit $r \to \infty$, stating any assumptions.

[2 marks]