PX2132 Introductory Quantum Mechanics

Problems

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All videos are available on the youtube channel Introductory Quantum Mechanics (link available at felixflicker.com/teaching, or on Learning Central).

The number of marks assigned to each question is provided to give an idea of how long should be spent on each question. The 2020 exam totalled 80 marks and took 2 hours.

Questions should be submitted via turnitin by the specified date, or handed in during the Tuesday class each week.

0. Vectors, matrices, and differential equations

28 marks total.

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0.1 Eigenvalues and eigenvectors

The Pauli matrices are defined to be

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \; \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1}$$

0.1.1

Find the eigenvalues and normalized eigenvectors of each Pauli matrix.

[5 marks]

0.1.2

Show that each matrix squares to the identity.

[1 mark]

0.1.3

Show that each matrix is its own inverse.

[1 mark]

0.1.4

The 'commutator' of two matrices A and B is defined as

$$[A, B] \triangleq AB - BA \tag{2}$$

where $\triangleq$ indicates that this is a definition. Show that

$$\left[\frac{1}{2}\sigma_x, \frac{1}{2}\sigma_y\right] = \frac{i}{2}\sigma_z. \tag{3}$$

[3 marks]

0.2 The wave equation

The one-dimensional wave equation is a partial differential equation (PDE):

$$\left(\frac{\partial^2 u(x,t)}{\partial t^2}\right)_x = c^2 \left(\frac{\partial^2 u(x,t)}{\partial x^2}\right)_t \tag{4}$$

where the subscripts indicate what is held constant in each case. You should have seen it already in the first year, although it may not have been examinable. It will provide some important intuition when we study the Schr¨dinger equation in quantum mechanics.

0.2.1

Substituting the ansatz

$$u(x,t) = \phi(x)\, T(t) \tag{5}$$

show that the equation can be separated into two ordinary differential equations (ODEs):

$$\frac{1}{c^2}\frac{1}{T(t)}\frac{\mathrm{d}^2 T(t)}{\mathrm{d}t^2} = \frac{1}{\phi(x)}\frac{\mathrm{d}^2\phi(x)}{\mathrm{d}x^2}. \tag{6}$$

[4 marks]

0.2.2

Since both sides are equal for all t and x they must be equal to the same constant. Calling this constant $-\lambda^2$, Eq. 6 now splits into two equations:

$$\frac{1}{c^2}\frac{1}{T(t)}\frac{\mathrm{d}^2 T(t)}{\mathrm{d}t^2} = -\lambda^2 \tag{7}$$

$$\frac{1}{\phi(x)}\frac{\mathrm{d}^2\phi(x)}{\mathrm{d}x^2} = -\lambda^2. \tag{8}$$

By solving these two equations separately, show that their general solutions take the form

$$T(t) = A\sin(c\lambda t) + B\cos(c\lambda t) \tag{9}$$

$$\phi(x) = C\sin(\lambda x) + D\cos(\lambda x). \tag{10}$$

[4 marks]

0.2.3

Say that Equation 4 is describing the motion of a string which is fixed at $x = 0$ and $x = L$. This implies the boundary conditions

$$\phi(0) = 0 \tag{11}$$

and

$$\phi(L) = 0. \tag{12}$$

Explain why this implies

(a) $D = 0$

[1 mark]

(b) $\lambda = n\pi/L$, with n a positive integer.

[2 marks]

0.2.4

Say the string is initially at rest, *i.e.*

$$\left(\frac{\partial u\left(x,t\right)}{\partial t}\right)_x\Bigg|_{t=0} = \dot{u}\left(x,0\right) = 0. \tag{13}$$

What value must A take?

[1 mark]

0.2.5

Putting all this together, show that the solutions to Eq 4 take the form

$$u_n\left(x,t\right) = a_n \cos\left(\frac{cn\pi t}{L}\right)\sin\left(\frac{n\pi x}{L}\right) \tag{14}$$

where a_n is a normalization constant. An n subscript has been added to u as a reminder that the wave function depends on n, which is takes integer values.

[3 marks]

0.2.6

Sketch these cases:

(a) $u_1(x,0)$

[1 mark]

(b) $u_1(x,L/2c)$

[1 mark]

(c) $u_2(x,0)$.

[1 mark]

1 Introduction to quantum mechanics

Satisfactory completion of this problem set is worth 1% of your total mark for the course. Satisfactory completion is defined as a meaningful attempt at every question, regardless of success. The number of marks is provided to give an idea of how long should be spent on each question. You have the videos, notes, and textbooks to help you.

Please submit your responses via turnitin no later than **11am on Tuesday 5th October**, or hand in answers at the start of the class that day.
Along with your answers please provide a 1-page cover sheet addressing the following points.

- Which questions did you find challenging?
- Give a brief statement as to where you got stuck in each case.
- State which resources you used to seek an answer in each case.
- Do you have any suggestions for improvement of this problem sheet?

30 marks total.

1.0 Videos

These questions cover content in videos: **V1.0, V1.1, V1.2, V1.3, V1.4, V1.5**.

1.1 Probability amplitudes

List three reasons why $\psi(x,t)$ is not suitable to interpret as a probability density, but $|\psi(x,t)|^2$ is.

[3 marks]

1.2 The Schrödinger equation

The time dependent Schrödinger equation (TDSE) is

$$i\hbar\partial_t\psi(x,t) = \hat{H}\psi(x,t)\,. \qquad (15)$$

1.2.1

In this course we will assume the Hamiltonian $\hat{H}$ has no explicit time dependence. By defining

$$\psi(x,t) = \phi(x)\,T(t) \qquad (16)$$

show that the TDSE is separable, *i.e.* it can be re-arranged to the form

$$\frac{i\hbar}{T(t)}\frac{\mathrm{d}T(t)}{\mathrm{d}t} = \frac{1}{\phi(x)}\hat{H}\phi(x)\,. \tag{17}$$

[3 marks]

1.2.2

Eq. 17 tells us that both sides of the equation must be equal to the same constant. Calling this constant E, derive the time independent Schrödinger equation (TISE):

$$\hat{H}\phi(x) = E\phi(x)\,. \tag{18}$$

[2 marks]

Why is E an appropriate label for this constant?

[1 mark]

1.2.3

Solve the corresponding equation for $T(t)$.

[3 marks]

1.2.4

Hence write down $\psi(x,t)$.

[1 mark]

1.3 Probability current density

1.3.1

The probability density is defined to be

$$\rho(x,t) = |\psi(x,t)|^2\,. \tag{19}$$

Use the TDSE to show that

$$\partial_t\rho + \partial_x j = 0 \tag{20}$$

where

$$j(x,t) = -\frac{i\hbar}{2m}\left(\psi^*\partial_x\psi - \psi\partial_x\psi^*\right). \tag{21}$$

[7 marks]

Interpret the result physically.

[2 marks]

1.3.2

A certain right-going plane wave takes the form

$$\psi(x,t) = \exp(i(kx - \omega t)). \tag{22}$$

Find the probability current density $j(x,t)$ for this right-going plane wave.

[4 marks]

1.3.3

(a) Using the de Broglie relation show that, in this simple case, j describes the velocity of the waves.

[2 marks]

(b) Why would you expect this physically?

[2 marks]

2 Scattering and tunnelling

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Please submit your responses via turnitin no later than **11am on Tuesday 12th October**, or hand in answers at the start of the class that day.
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- Which questions did you find challenging?
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- State which resources you used to seek an answer in each case.
- Do you have any suggestions for improvement of this problem sheet?

40 marks total.

2.0 Videos

These questions cover content in videos: **V2.1a, V2.1b, V2.1c, V2.1d, V2.2, V2.3**.

2.1 Scattering from a potential step

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

$$V(x) = \begin{cases} 0,\ x < 0\,(\text{region } I) \\ V_0,\ x \geq 0\,(\text{region } II). \end{cases} \tag{23}$$

2.1.1

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

$$\phi_I(x) = \exp(ikx) + r\exp(-ikx) \tag{24}$$

$$\phi_{II}(x) = t\exp(-\kappa x). \tag{25}$$

[2 marks]

2.1.2

Find expressions for k and κ in terms of E and V_0.

[3 marks]

2.1.3

State the two boundary conditions obeyed at the step.

[2 marks]

2.1.4

Find the reflection (r) and transmission (t) amplitudes.

[5 marks]

2.1.5

Using the probability current densities find the reflection (R) and transmission (T) probabilities.

[3 marks]

2.1.6

(a) Show that $R + T = 1$.

[1 mark]

(b) Why must this be the case?

[1 mark]

2.1.7

Sketch the waves in each region, paying attention to the amplitude, phase, and wavelength of the waves, for the following cases:
(a) $E \gg V_0$

[4 marks]

(b) $E \gtrsim V_0$.

[4 marks]

2.2 Scattering over a barrier

Consider the potential

$$V(x) = \begin{cases} 0,\ x < -L\,(\text{region 1}) \\ V_0,\ -L \leq x \leq L\,(\text{region 2}) \\ 0,\ x \geq L\,(\text{region 3}). \end{cases} \tag{26}$$

Assume $E > V_0$, and that a wave is incident from the left ($x = -\infty$). Define the solutions in each region to be

$$\phi_1 = \exp(ikx) + r\exp(-ikx) \tag{27}$$

$$\phi_2 = a\exp(ik'x) + b\exp(-ik'x) \tag{28}$$

$$\phi_3 = t\exp(-ikx)\,. \tag{29}$$

2.2.1

Sketch the potential.

[2 marks]

2.2.2

Identify the conditions on k and k' in terms of E and V_0.

[2 marks]

2.2.3

State the two boundary conditions at each end of the barrier.

[4 marks]

2.2.4

What is meant by 'resonant transmission'?

[1 mark]

2.2.5

The resonant transmission condition in this case is that $k'L = n\pi$ for integer n. On your sketch of the potential, add sketches of the wavefunctions of the two lowest-energy resonant states.

[3 marks]

2.2.6

Solving for the transmission probability gives the result

$$T = \frac{4E\left(E - V_0\right)}{4E\left(E - V_0\right) + V_0^2 \sin^2\left(L\sqrt{2m\left(E - V_0\right)}/\hbar\right)}. \tag{30}$$

For which energies is the barrier at resonance?

[2 marks]

3 Bound states (I)

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Please submit your responses via turnitin no later than **11am on Tuesday 19th October**, or hand in answers at the start of the class that day.
Along with your answers please provide a 1-page cover sheet addressing the following points.

- Which questions did you find challenging?
- Give a brief statement as to where you got stuck in each case.
- State which resources you used to seek an answer in each case.
- Do you have any suggestions for improvement of this problem sheet?

20 marks total.

3.0 Videos

Please watch videos: **V3.1, V3.2, V3.3, V3.4, V3.5.**

3.1 The infinite potential well

Consider the TISE

$$\left(-\frac{\hbar^2}{2m}\partial_x^2 + V\left(x\right)\right)\phi_n\left(x\right) = E_n\phi_n\left(x\right) \tag{31}$$

with the potential

$$V\left(x\right) = \begin{cases} 0, & -L/2 \le x \le L/2 \\ \infty, & \text{otherwise.} \end{cases} \tag{32}$$

3.1.1

Sketch the potential and the first four energy eigenfunctions.

[3 marks]

3.1.2

Which eigenfunctions $\phi_n\left(x\right)$ will be odd functions, and which even?

[1 mark]

Bearing this in mind will help simplify many of the remaining questions!

3.1.3

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]

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

[1 mark]

3.1.4

Write down the solutions to the TDSE, $\psi_n(x,t)$.

[2 marks]

3.1.5

Show that the probability density

$$\rho(x) = |\psi_n(x,t)|^2 \tag{33}$$

is time independent for all energy eigenfunctions.

[1 mark]

3.2 Infinite sets of bound states form an orthonormal basis

Whenever all the solutions of the TISE are bound states $\phi_n(x)$, these states must form an orthonormal basis:

$$\int_{-\infty}^{\infty} \phi_n^*(x)\,\phi_m(x)\,\mathrm{d}x = \delta_{nm} \tag{34}$$

where the Kronecker delta is defined as

$$\delta_{nm} = \begin{cases} 1,\ n = m \\ 0,\ \text{otherwise.} \end{cases}$$

Show that this implies that any function can be written as a sum of these energy eigenstates

$$f(x) = \sum_{n=1}^{\infty} f_n \phi_n(x) \tag{35}$$

by finding an expression for the coefficients f_n.

[5 marks]

4 Bound states (II)

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Please submit your responses via turnitin no later than **11am on Tuesday 26th October**, or hand in answers at the start of the class that day.
Along with your answers please provide a 1-page cover sheet addressing the following points.

- Which questions did you find challenging?
- Give a brief statement as to where you got stuck in each case.
- State which resources you used to seek an answer in each case.
- Do you have any suggestions for improvement of this problem sheet?

40 marks total.

4.0 Videos

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

4.1 Quantum superposition

Consider again the infinite well potential of Eq. 32, and the energy eigenvalues and normalized eigenvectors you found in question **3.1.3**.

4.1.1

Consider the state

$$\chi\left(x,t\right)=\mathcal{N}\left(3\psi_1\left(x,t\right)+4\psi_2\left(x,t\right)\right). \tag{36}$$

which is a quantum superposition of two energy eigenstates. What is the value of the normalization constant $\mathcal{N}$?

[2 marks]

4.1.2

(a) What are the possible outcomes of a measurement of the energy of state χ?

[2 marks]

(b) What are the probabilities of each outcome being found?

[2 marks]

4.1.3

Find the time-dependent probability density of $\chi(x,t)$.

[3 marks]

After how long does the state return to its original form?

[2 marks]

4.2 Deriving the time evolution of a state

Consider again the infinite well potential of Eq. 32, and the energy eigenvalues and normalized eigenvectors you found in question **3.1.3**.

Not all states are energy eigenstates. Consider a state described by a 'top hat function':

$$\varpi(x) = \begin{cases} (\alpha L)^{-1/2}, \; -\alpha\frac{L}{2} \le x \le \alpha\frac{L}{2} \\ 0, \text{ otherwise} \end{cases} \tag{37}$$

where $0 < \alpha \le 1$.

4.2.1

Sketch the potential and the state $\varpi(x)$.

[2 marks]

4.2.2

Check this state is normalised.

[2 marks]

4.2.3

In question 3.2 you showed that any function (meeting the boundary conditions) can be written as a weighted sum of energy eigenstates. Show that $\varpi(x)$ can be written as:

$$\varpi(x) = \sum_{n \text{ odd}} f_n \phi_n(x) \tag{38}$$

where

$$f_n = \sqrt{2\alpha}\,\mathrm{sinc}\left(\frac{n\pi\alpha}{2}\right). \tag{39}$$

[3 marks]

4.2.4

Therefore state the subsequent time evolution $\varpi(x,t)$.

[1 mark]

4.3 The finite potential well

Consider the potential

$$V(x) = \begin{cases} 0, \ x \leq -L & \text{(region 1)} \\ -V_0, \ -L < x < L & \text{(region 2)} \\ 0, \ L \leq x & \text{(region 3)} \end{cases} \tag{40}$$

and denote the solutions to the TISE in each region $\phi_i(x)$ with $i \in [1,3]$.

4.3.1

Sketch the potential and the three lowest-energy bound states, assuming three exist.

[4 marks]

4.3.2

State the two boundary conditions at each end of the well.

[4 marks]

4.3.3

(a) Assuming $E < 0$ the states can be written:

$$\phi_1(x) = A\exp(\kappa x) \tag{41}$$

$$\phi_2(x) = B\cos(kx) + C\sin(kx) \tag{42}$$

$$\phi_3(x) = D\exp(-\kappa x)\,. \tag{43}$$

Find expressions for κ and k as functions of energy.

[2 marks]

(b) Why must κ be the same in regions 1 and 3?

[1 mark]

(c) Why must the energy eigenstates be either symmetric or antisymmetric?

[1 mark]

State the constraints on the coefficients in each case.

[2 marks]

(d) Use the boundary conditions to find a constraint relating k and κ in both the symmetric and antisymmetric cases.

[2 marks]

(e) Show how you could go about solving these equations graphically (without actually doing so).

[2 marks]

(f) Prove there must always be at least one bound state in the well regardless of how small V_0 is.

[3 marks]

5 Finite-dimensional Hilbert spaces

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Please submit your responses via turnitin no later than **11am on Tuesday 2nd November**, or hand in answers at the start of the class that day.
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40 marks total.

5.0 Videos

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

5.1 Hermitian conjugate

5.1.1

Define a complex N-dimensional vector

$$|v\rangle = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_N \end{pmatrix}. \tag{44}$$

(a) Look up the axioms defining a linear vector space. State them here, using this new notation. Use this new notation in the following questions.

[3 marks]

Write expressions for:
(b) the complex conjugate $(|v\rangle)^*$

[1 mark]

(c) the transpose $(|v\rangle)^T$.

[1 mark]

(d) What are the matrix dimensions of each object?

[2 marks]

5.1.2

Show that $\left((|v\rangle)^T\right)^* = \left((|v\rangle)^*\right)^T$.

[2 marks]

N.B The relevance is that we can therefore write $(|v\rangle)^{T*}$ without ambiguity. This is called the Hermitian conjugate $(|v\rangle)^\dagger$:

$$(|v\rangle)^\dagger \triangleq (|v\rangle)^{T*} . \tag{45}$$

By convention we write this

$$(|v\rangle)^\dagger \triangleq \langle v|. \tag{46}$$

5.2 Inner product

5.2.1

Show that the inner product $\langle u||v\rangle$, which we conventionally write $\langle u|v\rangle$, is a complex scalar.

[2 marks]

5.2.2

Show that

$$(\langle u|v\rangle)^* = \langle v|u\rangle. \tag{47}$$

[2 marks]

5.2.3

Show that the norm of $|v\rangle$, *i.e.* its length, denoted $\||v\rangle\|$, is given by

$$\||v\rangle\| = \sqrt{\langle v|v\rangle}. \tag{48}$$

[2 marks]

5.2.4

Let

$$|v\rangle = \alpha|u\rangle + \beta|w\rangle \tag{49}$$

with complex α and β. Assuming $|u\rangle$ and $|w\rangle$ are orthogonal and normalised, find a condition on α and β for $|v\rangle$ to also be normalised.

[2 marks]

5.3 Matrices acting on vectors

Assume A is an $N \times N$ complex matrix, and $|u\rangle$ and $|v\rangle$ are N-dimensional complex vectors. State the dimensions of the following objects:

5.3.1 $A|v\rangle$

[1 mark]

5.3.2 $\langle v|A$

[1 mark]

5.3.3 $\langle u|A|v\rangle$**.**

[1 mark]

5.4 Outer product

In general we denote the outer product (also called the tensor product) between two N-dimensional vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ as

$$\boldsymbol{u} \otimes \boldsymbol{v} \triangleq \boldsymbol{u}\boldsymbol{v}^\dagger.$$

Element-wise the statement is that

$$[\boldsymbol{u} \otimes \boldsymbol{v}]_{ij} = u_i v_j^*$$

(*i.e.* multiply element-by-element).

In general the vectors need not be the same length, but we will assume they are.

(a) Thinking again of N-dimensional vectors as $N \times 1$ matrices, explain why the outer product is an $N \times N$ matrix.

[1 mark]

(b) Show that $|v\rangle\langle u|$ is an outer product.

[2 marks]

5.5 Resolution of the identity

Assume $|e_i\rangle$ ($i \in [1, N]$) form a complete orthonormal basis.
(a) What is $\langle e_i|e_j\rangle$?

[1 mark]

(b) For an arbitrary vector $|v\rangle$ with elements v_i explain why

$$|v\rangle = \sum_{i=1}^{N} v_i|e_i\rangle \tag{50}$$

where

$$v_i = \langle e_i|v\rangle. \tag{51}$$

[2 marks]

(c) Two matrices A and B are equivalent iff

$$\langle u|A|v\rangle = \langle u|B|v\rangle \tag{52}$$

for all $|u\rangle$, $|v\rangle$. Using the results of (b) prove the *resolution of the identity*

$$\mathbb{I} = \sum_{i=1}^{N} |e_i\rangle\langle e_i| \tag{53}$$

where $\mathbb{I}$ is the $N \times N$ identity matrix.

[3 marks]

5.6 Matrices and eigenvalues

5.6.1

Using the resolution of the identity, show that any Hermitian matrix M can be written in the following form:

$$M = \sum_{i=1}^{N} \lambda_i|i\rangle\langle i| \tag{54}$$

where

$$M|i\rangle = \lambda_i|i\rangle. \tag{55}$$

[3 marks]

5.6.2

Show this explicitly for each of the three Pauli matrices (you found the eigenvalues and normalised eigenvectors in question 0.4.1):

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{56}$$

[3 marks]

5.7 Spin-1/2

5.7.1

The spin operators are defined to be

$$\hat{S}_i = \frac{\hbar}{2}\sigma_i \tag{57}$$

with $i = x, y, z$. Show that each of the three spin operators has eigenvalues $\pm\hbar/2$ and find the corresponding normalised eigenvectors (you found the eigenvalues and normalised eigenvectors in question 0.4.1).

[3 marks]

5.7.2

Denote the eigenvector of $\hat{S}_i$ with eigenvalue $+\hbar/2$ with the symbol $|\uparrow_i\rangle$, and that with eigenvalue $-\hbar/2$ with the symbol $|\downarrow_i\rangle$:

$$\hat{S}_i|\uparrow_i\rangle = \frac{\hbar}{2}|\uparrow_i\rangle \tag{58}$$

$$\hat{S}_i|\downarrow_i\rangle = -\frac{\hbar}{2}|\downarrow_i\rangle. \tag{59}$$

Using the result of equation 54 explain why each spin operator can be written in the form

$$\hat{S}_i = \frac{\hbar}{2}\left(|\uparrow_i\rangle\langle\uparrow_i| - |\downarrow_i\rangle\langle\downarrow_i|\right).$$

[2 marks]

6 Operators and observables

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Along with your answers please provide a 1-page cover sheet addressing the following points.

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- State which resources you used to seek an answer in each case.
- Do you have any suggestions for improvement of this problem sheet?

40 marks total.

6.0 Videos

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

6.1 The Heisenberg picture

In the Heisenberg picture states $|\psi\rangle$ are time-independent, but operators are time dependent:

$$\hat{A}_H(t) = \exp\left(i\hat{H}t/\hbar\right)\hat{A}_S \exp\left(-i\hat{H}t/\hbar\right). \tag{60}$$

Here $\hat{A}_H(t)$ is a time-dependent operator in the Heisenberg picture and $\hat{A}_S$ is a time-independent operator in the Schrödinger picture (*e.g.* $\hat{x}$). Similarly, in the Schrödinger picture states are time dependent:

$$|\psi_S(t)\rangle = \exp\left(-i\hat{H}t/\hbar\right)|\psi_S(0)\rangle = \exp\left(-i\hat{H}t/\hbar\right)|\psi_H\rangle \tag{61}$$

where $|\psi_S(t)\rangle$ is a time-dependent state in the Schrödinger picture and $|\psi_H\rangle$ is a time-independent state in the Heisenberg picture, and an arbitrary choice of global phase has been made to set the two states equal at $t = 0$.

6.1.1

Two matrices or operators $\hat{A}$ and $\hat{B}$ are equivalent iff

$$\langle\varphi|\hat{A}|\psi\rangle = \langle\varphi|\hat{B}|\psi\rangle \quad \forall|\varphi\rangle,\, |\psi\rangle. \tag{62}$$

Show that

$$\langle\varphi_H|\hat{A}_H\left(t\right)|\psi_H\rangle = \langle\varphi_S\left(t\right)|\hat{A}_S|\psi_S\left(t\right)\rangle \tag{63}$$

and hence the two pictures are equivalent.

[2 marks]

6.1.2

(a) Using the TDSE explain why the differential operator $i\hbar\partial_t$ must commute with the Hamiltonian $\hat{H}$:

$$\left[i\hbar\partial_t, \hat{H}\right] = 0. \tag{64}$$

[1 mark]

(b) Why must

$$\left[\hat{H}, f\left(\hat{H}\right)\right] = 0 \tag{65}$$

for any function f?

[2 marks]

6.1.3

By taking the partial derivative of Eq. 60 with respect to time, and using the previous results, derive the Heisenberg equation of motion:

$$i\hbar\frac{\mathrm{d}\hat{A}_H\left(t\right)}{\mathrm{d}t} = \left[\hat{A}_H\left(t\right), \hat{H}\right]. \tag{66}$$

[4 marks]

6.1.4

Use this result to prove Ehrenfest's theorem:

$$i\hbar\frac{\mathrm{d}\langle\hat{A}\rangle}{\mathrm{d}t} = \langle\left[\hat{A}, \hat{H}\right]\rangle. \tag{67}$$

[4 marks]

6.2 The Heisenberg Uncertainty Principle

6.2.1

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

[2 marks]

6.2.2

The *canonical commutation relation* (an experimentally-derived result which you should memorise!) is

$$[\hat{x}, \hat{p}] = i\hbar\hat{\mathbb{I}}. \tag{68}$$

Here $\hat{\mathbb{I}}$ is the identity operator, for which any state is an eigenstate with with eigenvalue 1. Use this to find the Heisenberg uncertainty relation between the position and momentum of a particle.

[2 marks]

6.2.3

Using the commutation relation between spin operators:

$$\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\hat{S}_z \tag{69}$$

find the uncertainty relation between the x- and y- components of the intrinsic angular momentum.

[2 marks]

6.2.4

Give a physical explanation for the mathematical results you just derived which you would be willing to defend to your classmates. You may wish to think about which interpretation of quantum mechanics (if any) you subscribe to.

[2 marks]

6.3 Joint eigenvectors

In this question we will prove that if two matrices commute they have a joint set of eigenvectors.

6.3.1

Consider two matrices A and B which have all the same eigenvectors but potentially different eigenvalues:

$$A|v_n\rangle = a_n|v_n\rangle \tag{70}$$

$$B|v_n\rangle = b_n|v_n\rangle. \tag{71}$$

Assuming that neither A nor B has a zero eigenvalue, show that

$$[A, B] = 0. \tag{72}$$

[2 marks]

6.3.2

Now we'll prove the converse. Define the eigenvectors of A to be

$$A|a_n\rangle = a_n|a_n\rangle. \tag{73}$$

Show that if

$$[A, B] = 0 \tag{74}$$

then $|a_n\rangle$ must also be an eigenvector of B.

[5 marks]

6.3.3

Explain why these results show that if two quantum mechanical observables can be known simultaneously their operators must commute, and vice versa.

[2 marks]

6.4 Quantum numbers

6.4.1

Explain what is meant by a quantum number.

[2 marks]

6.4.2

Using Ehrenfest's theorem, explain why, if the operator describing an observable commutes with the Hamiltonian, then the observable corresponds to a good quantum number.

[4 marks]

6.4.3

Hence explain why energy is always a good quantum number.

[2 marks]

6.4.4

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

[2 marks]

7 Quantum mechanics

Satisfactory completion of this problem set is worth 1% of your total mark for the course. Satisfactory completion is defined as a meaningful attempt at every question, regardless of success. The number of marks is provided to give an idea of how long should be spent on each question. You have the videos, notes, and textbooks to help you.

Please submit your responses via turnitin no later than **11am on Tuesday 16th November**, or hand in answers at the start of the class that day.
Along with your answers please provide a 1-page cover sheet addressing the following points.

- Which questions did you find challenging?
- Give a brief statement as to where you got stuck in each case.
- State which resources you used to seek an answer in each case.
- Do you have any suggestions for improvement of this problem sheet?

20 marks total.

7.0 Videos

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

7.1 Infinite-dimensional Hilbert spaces

7.1.1

State the axioms of a linear vector space.

[3 marks]

Show that these axioms are satisfied by complex functions $f(x)$.

[3 marks]

We are therefore justified in using vector notation to decribe functions: $|f\rangle$, or, in the position basis specifically, $\langle x|f\rangle = f(x)$.

7.1.2

State the axioms of an 'inner product space'.

[1 mark]

Working in the position basis $f(x) = \langle x|f\rangle$ show that the axioms are satisfied by complex functions if the inner product is defined as

$$\langle f|g\rangle \triangleq \int_{-\infty}^{\infty} f(x)^* g(x)\,\mathrm{d}x. \tag{75}$$

[3 marks]

7.1.3

Explain why the norm of any quantum state $|\psi\rangle$ must be one.

[1 mark]

State this restriction in terms of the wavefunction $\langle x|\psi\rangle = \psi(x)$.

[1 mark]

This last property, square-integrability, defines the space of wavefunctions to be an infinite-dimensional Hilbert space.

7.2 Hermiticity of differential operators

7.2.1

State the condition for a differential operator $\hat{A}$ (written in the position basis) to be Hermitian.

[2 marks]

7.2.2

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]

(b) ∂_x

[1 mark]

(c) $-i\hbar\partial_x$

[1 mark]

(d) ∂_x^2

[1 mark]

(e) $-i\hbar(x\partial_y - y\partial_x)$

[1 mark]

(f) ∇

[1 mark]

8 The quantum harmonic oscillator

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- State which resources you used to seek an answer in each case.
- Do you have any suggestions for improvement of this problem sheet?

30 marks total.

8.0 Videos

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

8.1 Choosing units

The Hamiltonian for the quantum harmonic oscillator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2. \tag{76}$$

8.1.1

Working in the position basis, letting

$$x = \alpha y \tag{77}$$

show that the TISE can be written

$$-\frac{1}{2}\frac{\mathrm{d}^2\phi_n\left(y\right)}{\mathrm{d}y^2} + \frac{1}{2}y^2\phi_n\left(y\right) = \epsilon_n\phi_n\left(y\right) \tag{78}$$

where y and ϵ_n are quantities you should define.

[2 marks]

8.2 Ladder operators 1: building the ladder

8.2.1

Continuing with the rescaled variable from the previous question, the Hamiltonian in the position basis is

$$\hat{H} = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}y^2} + \frac{1}{2}y^2. \tag{79}$$

Defining the lowering operator

$$\hat{a} = \frac{1}{\sqrt{2}}\left(y + \frac{\mathrm{d}}{\mathrm{d}y}\right) \tag{80}$$

and the raising operator

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(y - \frac{\mathrm{d}}{\mathrm{d}y}\right) \tag{81}$$

show Eq. 79 can be rewritten as

$$\hat{H} = \hat{a}^\dagger\hat{a} + \frac{1}{2}\hat{\mathbb{I}}. \tag{82}$$

[4 marks]

8.2.2

Show that

$$\left[\hat{a}, \hat{a}^\dagger\right] = \hat{\mathbb{I}}. \tag{83}$$

[3 marks]

8.2.3

Show that

$$\left[\hat{a}^\dagger, \hat{H}\right] = -\hat{a}^\dagger. \tag{84}$$

[3 marks]

8.2.4

By acting on both sides of the time-independent Schrödinger equation

$$\hat{H}\phi_n(y) = \epsilon_n \phi_n(y) \tag{85}$$

with $\hat{a}^\dagger$, show that

$$\hat{H}\left(\hat{a}^\dagger \phi_n(y)\right) = (\epsilon_n + 1)\left(\hat{a}^\dagger \phi_n(y)\right).$$

[4 marks]

8.2.5

Explain how the previous result proves that the harmonic oscillator has an infinite ladder of energy eigenstates evenly-spaced in energy.

[2 marks]

8.3 Ladder operators 2: states

8.3.1

The eigenstate on the lowest rung of the ladder must obey this condition:

$$\hat{a}\phi_0(y) = 0. \tag{86}$$

Use this equation to solve for the normalised eigenstate $\phi_0(y)$ and the corresponding energy eigenvalue ϵ_0.

[4 marks]

8.3.2

Find the normalised first excited state and the corresponding energy eigenvalue.

[5 marks]

8.4 Second quantisation

Explain what is meant by second quantisation.

[3 marks]

9 The Schrödinger equation in three dimensions

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Please submit your responses via turnitin no later than **11am on Tuesday 30th November**, or hand in answers at the start of the class that day.
Along with your answers please provide a 1-page cover sheet addressing the following points.

- Which questions did you find challenging?
- Give a brief statement as to where you got stuck in each case.
- State which resources you used to seek an answer in each case.
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30 marks total.

9.0 Videos

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

9.1

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

$$V(\boldsymbol{r}) = \begin{cases} 0, & 0 \le r_i \le L \\ \infty, & \text{otherwise} \end{cases} \tag{87}$$

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

9.1.1

Sketch the potential.

[1 mark]

9.1.2

Write down the time-independent Schrödinger equation for this potential.

[1 mark]

9.1.3

Noting that the equation is separable in x, y, and z, find the energy eigenvalues and normalised energy eigenstates.

[7 marks]

9.1.4

The degeneracy of an energy eigenstate is the number of other energy eigenstates with the same energy eigenvalue. Find the degeneracy of the lowest five energy levels of the 3D infinite potential well.

[5 marks]

9.1.5

Imagine the well's shape is cuboidal instead of cubic. What would be the degeneracy of the lowest five energy levels in this case?

[3 mark]

9.2 Angular momentum operators

9.2.1

State the commutation relation between any two angular momentum operators.

[1 mark]

Show that

$$\left[\hat{L}^2, \hat{L}_z\right] = 0. \tag{88}$$

[3 marks]

9.2.2

Denote the eigenstates of $\hat{L}_z$ and $\hat{L}^2$ as follows:

$$\hat{L}^2|l\rangle = \hbar^2 l\,(l+1)\,|l\rangle \tag{89}$$

$$\hat{L}_z|m\rangle = \hbar m|m\rangle \tag{90}$$

where l and m are integers. Why is it reasonable to write a state such as $|l, m\rangle$ labelled by both eigenvalues?

[2 marks]

9.2.3

Defining

$$\hat{L}_{\pm} = \hat{L}_x \pm i\hat{L}_y \tag{91}$$

show that

$$\left[\hat{L}_{\pm}, \hat{L}_z\right] = \mp\hbar\hat{L}_{\pm}. \tag{92}$$

[3 marks]

9.2.4

Using the reasoning you developed with the quantum harmonic (energy) ladder operators, explain why the previous result defines $\hat{L}_{\pm}$ to be angular momentum raising and lowering operators.

[4 marks]

10 The Hydrogen Atom

Satisfactory completion of this problem set is worth 1% of your total mark for the course. Satisfactory completion is defined as a meaningful attempt at every question, regardless of success. The number of marks is provided to give an idea of how long should be spent on each question. You have the videos, notes, and textbooks to help you.

Please submit your responses via turnitin no later than **11am on Tuesday 7th December**, or hand in answers at the start of the class that day.
Along with your answers please provide a 1-page cover sheet addressing the following points.

- Which questions did you find challenging?
- Give a brief statement as to where you got stuck in each case.
- State which resources you used to seek an answer in each case.
- Do you have any suggestions for improvement of this problem sheet?

20 marks total.

10.1 The Bohr model

10.1.1

Write down the assumptions going into Bohr's (incorrect) model of the electronic states in the atom. Write a mathematical expression encoding Bohr's statement regarding the quantization of angular momentum.

[3 marks]

10.1.2

The energy levels of the atom in the Bohr model are:

$$E_n = \frac{m_e e^4}{2\left(4\pi\epsilon_0\right)^2 \hbar^2 n^2}. \tag{93}$$

Use this formula to calculate the ionization energy of hydrogen.

[3 marks]

10.1.3

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

[1 mark]

10.2 Spherically symmetric potentials

For polar co-ordinates

$$\boldsymbol{r} = (r, \theta, \phi) \tag{94}$$

The TISE reads

$$\hat{H}\psi(\boldsymbol{r}, t) = E\psi(\boldsymbol{r}, t) \tag{95}$$

where

$$\hat{H} = -\frac{\hbar^2}{2\mu r^2}\partial_r\left(r^2\partial_r\right) + \frac{1}{2\mu r^2}\hat{L}^2 + V(\boldsymbol{r}) \tag{96}$$

and

$$\hat{L}^2 = -\hbar^2\left(\frac{1}{\sin(\theta)}\partial_\theta\left(\sin(\theta)\,\partial_\theta\right) + \frac{1}{\sin^2(\theta)}\partial_\phi^2\right). \tag{97}$$

The symbol μ here is used in place of m for the mass of the particle.

10.2.1

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

[1 mark]

10.2.2

Explain why, if the potential is spherically symmetric, the TISE is separable using the ansatz

$$\psi(\boldsymbol{r}, t) = T(t)\,R(r)\,Y(\theta, \phi). \tag{98}$$

[2 marks]

10.2.3

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

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

and angular equation

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

[4 marks]

10.3 Radial equation

Explain why the results found for the angular equation tell us that the radial equation now takes the form

$$\hbar^2 \frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \frac{\mathrm{d}}{\mathrm{d}r}\right) R_l(r) + 2mr^2 (E - V) R_l(r) = \hbar^2 l(l+1) R_l(r) \tag{99}$$

giving an expression relating k and l.

[2 marks]

10.4 The hydrogen atom

10.4.1

Explain why the TISE of the electron in the hydrogen atom takes the form

$$\left(-\frac{\hbar^2}{2\mu r^2}\partial_r\left(r^2\partial_r\right) + \frac{\hbar^2 l(l+1)}{2\mu r^2} - \frac{e^2}{4\pi\epsilon_0 r}\right)\varphi_{n,l,m}(\boldsymbol{r}) = E_n\varphi_{n,l,m}(\boldsymbol{r}) \tag{100}$$

explaining the meaning of μ.

[4 marks]