PX2132 Introductory Quantum Mechanics

Problems and Answers

F. Flicker

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0. Vectors, matrices, and differential equations

Bring solutions along to the class at 10am on 5/10/20.

Most of these questions are intended as a review of first-year topics, but some new content will be introduced, indicated by *.

0.1 * Linear vector spaces

You will have seen various methods of writing vectors, such as $\boldsymbol{v}$, $\underline{v}$, $\overrightarrow{v}$. A particularly convenient notation for complex vectors, which we will use in this course, is $|v\rangle$. Define the N-dimensional vector $|v\rangle$ by

$$|v\rangle = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_N \end{pmatrix}. \tag{1}$$

Note that an N-dimensional vector is an $N \times 1$ matrix.

0.1.1 *

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

0.2 Matrix products

0.2.1

For the matrix

$$M = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \tag{2}$$

show that the eigenvalues are φ and $-\varphi^{-1}$ where $\varphi = \left(1+\sqrt{5}\right)/2$ is the golden ratio. Find the normalized eigenvectors.

ANS:

eigenvectors:

$$\frac{1}{\sqrt{3-\varphi}}\begin{pmatrix} 1 \\ \varphi - 1 \end{pmatrix}, \quad \frac{1}{\sqrt{3-\varphi}}\begin{pmatrix} \varphi - 1 \\ -1 \end{pmatrix}.$$

0.2.2

Show that

$$M^{-1} = \begin{pmatrix} 0 & 1 \\ 1 & -1 \end{pmatrix}. \tag{3}$$

0.2.3

Prove by induction that

$$M^n = \begin{pmatrix} F_{n+1} & F_n \\ F_n & F_{n-1} \end{pmatrix} \tag{4}$$

for $n > 1$, where

$$\begin{aligned} F_n &= 1,\ 1,\ 2,\ 3,\ 5,\ 8,\ 13,\ \ldots \\ n &= 1,\ 2,\ 3,\ 4,\ 5,\ 6,\ 7,\ \ldots \end{aligned} \tag{5}$$

are the Fibonacci numbers defined by $F_{n+1} = F_n + F_{n-1}$ for $n > 1$.

ANS:

$$M^2 = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} F_3 & F_2 \\ F_2 & F_1 \end{pmatrix} \checkmark$$

$$M^{n+1} = MM^n = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} M^n_{11} & M^n_{12} \\ M^n_{21} & M^n_{22} \end{pmatrix} = \begin{pmatrix} M^n_{11} + M^n_{21} & M^n_{12} + M^n_{22} \\ M^n_{11} & M^n_{12} \end{pmatrix}$$

$$\begin{pmatrix} M^{n+1}_{11} & M^{n+1}_{12} \\ M^{n+1}_{21} & M^{n+1}_{22} \end{pmatrix} = \begin{pmatrix} M^n_{11} + M^{n-1}_{11} & M^n_{12} + M^{n-1}_{12} \\ M^n_{11} & M^n_{12} \end{pmatrix}$$

$$= \begin{pmatrix} M^n_{11} + M^{n-1}_{11} & M^n_{12} + M^{n-1}_{12} \\ M^{n-1}_{11} + M^{n-2}_{11} & M^{n-1}_{12} + M^{n-2}_{12} \end{pmatrix}$$

therefore elements (1,1) and (1,2) obey straightforward Fibonacci relations, while elements (2,1) and (2,2) take the form of the Fibonacci number one earlier in the sequence than the entry above them.

0.3 Matrix transpose

For two square matrices A and B prove that

$$(AB)^T = B^T A^T. \tag{6}$$

ANS:

$$\begin{aligned}
([AB]_{ik})^T &= [AB]_{ki} \\
&= \sum_j A_{kj} B_{ji} \\
&= \sum_j B_{ji} A_{kj} \\
&= \sum_j B^T_{ij} A^T_{jk} \\
&= [B^T A^T]_{ik} .
\end{aligned}$$

0.4 Eigenvalues and eigenvectors

The Pauli matrices are defined to be

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \; \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{7}$$

0.4.1

Find the eigenvalues and eigenvectors of each.

ANS:

eigenvalues ± 1.

$$\begin{aligned}
\sigma_x &: \; \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \\
\sigma_y &: \; \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ -1 \end{pmatrix} \\
\sigma_z &: \; \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}
\end{aligned}$$

0.4.2

Show that each matrix squares to the identity.

0.4.3

Show that each matrix is its own inverse.

0.4.4 *

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

$$[A, B] \triangleq AB - BA \tag{8}$$

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

$$\left[\frac{1}{2}\sigma_x, \frac{1}{2}\sigma_y\right] = i\frac{1}{2}\sigma_z. \tag{9}$$

ANS:

$$\begin{aligned}
\left[\frac{1}{2}\sigma_x, \frac{1}{2}\sigma_y\right] &= \frac{1}{4}\left(\sigma_x\sigma_y - \sigma_y\sigma_x\right) \\
&= \frac{1}{4}\left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right) \\
&= \frac{1}{4}\left(\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}\right) \\
&= \frac{1}{2}\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \\
&= i\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = i\frac{1}{2}\sigma_z
\end{aligned}$$

0.5 Determinants

0.5.1

List the rules for simplifying determinants.

ANS:

- any row or column can be interchanged
- any multiple of any row or column can be added to any other
- the matrix can be transposed
- multiplying a row by a number multiplies the determinant by the same
- if any row or column is equal to any other the answer is zero

0.5.2

Show that the determinant of the matrix

$$M = \begin{pmatrix} -1 & 1 & 1 & 0 \\ 1 & \theta & -\theta & 0 \\ 0 & e^{ix} & e^{-ix} & -1 \\ 0 & \theta e^{ix} & -\theta e^{-ix} & -1 \end{pmatrix} \tag{10}$$

is

$$\det(M) = 4\theta\cos(x) - 2i\left(1+\theta^2\right)\sin(x)\,. \tag{11}$$

This is used when proving a result you will see when studying quantum tunnelling.

ANS:

(for example):

$$\begin{aligned}
\begin{vmatrix} -1 & 1 & 1 & 0 \\ 1 & \theta & -\theta & 0 \\ 0 & e^{ix} & e^{-ix} & -1 \\ 0 & \theta e^{ix} & -\theta e^{-ix} & -1 \end{vmatrix} &= -\begin{vmatrix} \theta & -\theta & 0 \\ e^{ix} & e^{-ix} & -1 \\ \theta e^{ix} & -\theta e^{-ix} & -1 \end{vmatrix} - \begin{vmatrix} 1 & 1 & 0 \\ e^{ix} & e^{-ix} & -1 \\ \theta e^{ix} & -\theta e^{-ix} & -1 \end{vmatrix} \\
&= -\begin{vmatrix} 0 & -\theta & 0 \\ 2\cos(x) & e^{-ix} & -1 \\ 2i\theta\sin(x) & -\theta e^{-ix} & -1 \end{vmatrix} - \begin{vmatrix} 0 & 1 & 0 \\ 2i\sin(x) & e^{-ix} & -1 \\ 2\theta\cos(x) & -\theta e^{-ix} & -1 \end{vmatrix} \\
&= -\begin{vmatrix} 0 & 2\cos(x) & 2i\theta\sin(x) \\ -\theta & e^{-ix} & -\theta e^{-ix} \\ 0 & -1 & -1 \end{vmatrix} - \begin{vmatrix} 0 & 2i\sin(x) & 2\theta\cos(x) \\ 1 & e^{-ix} & -\theta e^{-ix} \\ 0 & -1 & -1 \end{vmatrix} \\
&= -\theta\begin{vmatrix} 2\cos(x) & 2i\theta\sin(x) \\ -1 & -1 \end{vmatrix} + \begin{vmatrix} 2i\sin(x) & 2\theta\cos(x) \\ -1 & -1 \end{vmatrix} \\
&= 2\theta\cos(x) - 2i\theta^2\sin(x) - 2i\sin(x) + 2\theta\cos(x) \\
&= 4\theta\cos(x) - 2i\left(1+\theta^2\right)\sin(\theta)\,.
\end{aligned}$$

0.5.3

Find element $(1,4)$ of the inverse matrix M^{-1}, *i.e.* M^{-1}_{14}. Note that you do not need to compute the entire inverse matrix to do this.

ANS:

$M^{-1}_{14} = C_{41}/\det(M)$ where C is the matrix of signed cofactors. That is, the determinant of the 3x3 matrix formed by deleting row 4 and column 1. The sign of cofactor (4,1) is -. Therefore

$$
\begin{aligned}
M^{-1}_{14} &= \frac{1}{\det(M)} \begin{vmatrix} 1 & 1 & 0 \\ \theta & -\theta & 0 \\ e^{ix} & e^{-ix} & -1 \end{vmatrix} \\
&= \frac{1}{\det(M)} \begin{vmatrix} 1 & \theta & e^{ix} \\ 1 & -\theta & e^{-ix} \\ 0 & 0 & -1 \end{vmatrix} \\
&= \frac{1}{\det(M)} \begin{vmatrix} -\theta & e^{-ix} \\ 0 & -1 \end{vmatrix} - \frac{1}{\det(M)} \begin{vmatrix} \theta & e^{ix} \\ 0 & -1 \end{vmatrix} \\
&= \frac{2\theta}{\det(M)} \\
&= \frac{\theta}{2\theta\cos(x) - i(1+\theta^2)\sin(x)}.
\end{aligned}
$$

0.6 Separable PDEs

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

$$\left(\frac{\partial^2 u(x,t)}{\partial t^2}\right)_x = c^2 \left(\frac{\partial^2 u(x,t)}{\partial x^2}\right)_t \tag{12}$$

where the subscripts indicate what is held constant in each case.

0.6.1

Substituting the ansatz

$$u(x,t) = \phi(x)\,T(t) \tag{13}$$

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

$$\frac{1}{c^2}\frac{1}{T(t)}\frac{\mathrm{d}^2 T(t)}{\mathrm{d}t^2} = \frac{1}{\phi(x)}\frac{\mathrm{d}^2\phi(x)}{\mathrm{d}x^2}. \tag{14}$$

0.6.2

Since both sides are equal for all t and x they must be equal to the same constant. Calling this constant $-\lambda^2$ show that general solutions take the form

$$T(t) = A\sin(c\lambda t) + B\cos(c\lambda t) \tag{15}$$

$$\phi(x) = C\sin(\lambda x) + D\cos(\lambda x). \tag{16}$$

0.6.3

Say the equation is describing the motion of a string fixed at 0 and L. This implies the boundary conditions

$$\phi(0) = \phi(L) = 0. \tag{17}$$

Explain why this implies

(a) $D = 0$

ANS:

subtitute $x = 0$ into eq 16. and use $\phi(0) = 0$.

(b) $\lambda = n\pi/L$.

ANS:

with $D = 0$ already, substitute $x = L$ into eq 16. It could be that $C = 0$, but then $\phi(x) = 0$ for all x, which is incorrect. So instead $\sin(\lambda L) = 0$, which gives this condition (where n is an integer).

0.6.4

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

$$\left(\frac{\partial u(x,t)}{\partial t}\right)_x\bigg|_{t=0} = \dot{u}(x,0) = 0. \tag{18}$$

Show that the solutions take the form

$$u_n(x,t) = a_n\cos\left(\frac{cn\pi t}{L}\right)\sin\left(\frac{n\pi x}{L}\right) \tag{19}$$

where a_n is a normalization constant. Sketch the two lowest-energy solutions at a few key times.

ANS:

substituting the results of 0.6.3 we have the form

$$u(x,t) = C\left(A\sin\left(\frac{cn\pi t}{L}\right) + B\cos\left(\frac{cn\pi t}{L}\right)\right)\sin\left(\frac{n\pi x}{L}\right)$$

and now we require

$$0 = \dot{u}(x,0) = C\left(A\frac{cn\pi}{L}\right)\sin\left(\frac{n\pi x}{L}\right)$$

so $A = 0$. In principle the remaining coefficient BC can be a function of n (the integer labelling the different solutions). Relabel BC to a_n to get the requested form.

0.7 * Differential operators

Consider the partial derivative

$$\frac{\partial u(x,t)}{\partial t} \tag{20}$$

where the explicit statement as to which variables are held constant (*i.e.* x) has been omitted. A convenient trick is to consider the partial derivative to be an 'operator' $\partial/\partial t$ acting on the function $u(x,t)$:

$$\left(\frac{\partial}{\partial t}\right)u(x,t) \triangleq \frac{\partial u(x,t)}{\partial t}. \tag{21}$$

This can be abbreviated even further to

$$\partial_t u(x,t). \tag{22}$$

The utility of this notation derives from being able to write expressions such as

$$\left(\frac{\partial}{\partial t}\right)^2 = (\partial_t)^2 = \partial_t\partial_t = \partial_t^2. \tag{23}$$

You can always imagine the operator to be acting on some arbitrary function, as in Eq. 21, but it is often easier to work with the operators themselves. You have probably seen some differential operators before. For example, you may have seen the Laplace operator (Laplacian)

$$\triangle \triangleq \nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2 \tag{24}$$

or the d'Alembert operator (d'Alembertian):

$$\square \triangleq c^{-2}\partial_t^2 - \triangle = c^{-2}\partial_t^2 - \nabla^2. \tag{25}$$

0.7.1 *

Show that

$$\Box u = 0 \tag{26}$$

is a succinct way of writing the 3D wave equation.

ANS:

$$\begin{aligned}\Box u &= 0\\ \left(c^{-2}\partial_t^2 - \nabla^2\right) u &= 0\\ c^{-2}\partial_t^2 u - \nabla^2 u &= 0\\ \ddot{u} - c^2 u'' &= 0.\end{aligned}$$

0.7.2 *

By expanding the product show that the 1D wave equation can be written as

$$\left(\partial_t - c\partial_x\right)\left(\partial_t + c\partial_x\right) u\left(x,t\right) = 0. \tag{27}$$

ANS:

$$\left(\partial_t^2 - c^2\partial_x^2 + c\partial_t\partial_x - c\partial_x\partial_t\right) u\left(x,t\right) = 0$$

but

$$\partial_t\partial_x u = \partial_x\partial_t u$$

or, written out:

$$\frac{\partial^2 u}{\partial t\partial x} = \frac{\partial^2 u}{\partial x\partial t}$$

so

$$\left(\partial_t^2 - c^2\partial_x^2\right) u\left(x,t\right) = 0.$$

0.7.3 *

Show that the 1D wave equation can also be written as

$$(\partial_t + c\partial_x)(\partial_t - c\partial_x)\, u(x,t) = 0. \tag{28}$$

0.7.4 *

Operators, like matrices, may also fail to commute. Using the definition of the commutator in Eq. 8, along with Eqs. 27 and 28, deduce that the operators $\partial_t + c\partial_x$ and $\partial_t - c\partial_x$ commute:

$$[(\partial_t + c\partial_x), (\partial_t - c\partial_x)]\, u(x,t) = 0 \quad \forall \quad u. \tag{29}$$

ANS:

we have show that

$$(\partial_t - c\partial_x)(\partial_t + c\partial_x)\, u(x,t) = (\partial_t + c\partial_x)(\partial_t - c\partial_x)\, u(x,t)$$

and so

$$((\partial_t - c\partial_x)(\partial_t + c\partial_x) - (\partial_t + c\partial_x)(\partial_t - c\partial_x))\, u(x,t) = 0$$

which, by the definition of the determinant, is

$$[(\partial_t - c\partial_x), (\partial_t + c\partial_x)]\, u = 0.$$

Since u was not specified this holds for the operators themselves.

0.7.5 *

Define the variables $\eta = x - ct$ and $\nu = x + ct$.

Recall the chain rule:

$$\left(\frac{\partial f}{\partial \nu}\right)_\eta = \left(\frac{\partial x}{\partial \nu}\right)_\eta \left(\frac{\partial f}{\partial x}\right)_t + \left(\frac{\partial t}{\partial \nu}\right)_\eta \left(\frac{\partial f}{\partial t}\right)_x \tag{30}$$

which can be written as the following operators acting on f:

$$\partial_\nu = (\partial_\nu x)\,\partial_x + (\partial_\nu t)\,\partial_t. \tag{31}$$

(a) Show that

$$2c\partial_\eta = c\partial_x - \partial_t \tag{32}$$

$$2c\partial_\nu = c\partial_x + \partial_t. \tag{33}$$

(b) Therefore show that the wave equation in these co-ordinates reads

$$\partial_\eta \partial_\nu u(\eta, \nu) = 0. \tag{34}$$

ANS:

substitute eqns 32, 33 into eq 28.

(c) Deduce that a general solution to the wave equation can be written as

$$u(\eta, \nu) = f(\eta) + g(\nu) \tag{35}$$

or

$$u(x, t) = f(x - ct) + g(x + ct) \tag{36}$$

for arbitrary functions f and g.

(d) Interpret the result in terms of travelling waves.

ANS:

any solution to the wave equation can be written in terms of a right-going solution plus a left-going solution.

1 Introduction to quantum mechanics

Bring solutions along to the class at 10am on 5/10/20.

Questions marked # are beyond the syllabus. We may discuss them in the class if there is time.

Attempt all questions. Feel free to discuss with friends. Don't worry if you cannot answer a question fully as you will discuss the solutions in the class.

1.0 Videos

Please watch this week's videos: V1.0, V1.1, V1.2, V1.3, V1.4, V1.5.

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

1.1 Probability amplitudes

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

ANS:

- ψ is complex
- ψ depends on an arbitrary global phase
- conversely, when $|\psi|^2$ is integrated over all space it gives 1.

1.2 Quantum scales

A simple estimate as to whether quantum behaviour needs to be accounted for when modelling a physical system is provided by estimating a relevant quantity with the same units as $\hbar$. For example, an energy scale multiplied by a time scale, or a momentum scale multiplied by a length scale. If the quantity is significantly larger than $\hbar$ probably quantum effects can be neglected, otherwise they may be important. Estimate whether quantum effects are likely to be important in the following cases. You should be happy defending your answers to your classmates.

(a) A game of cricket

ANS:

e.g. momentum of ball $\sim 0.5\text{kg} \times 100\text{m/s} = 50\text{kgm/s}$, lengthscale $\sim 1\text{m}$, $px \sim 50 \gg 10^{-34}$. No.

(b) the behaviour of electrons in a transistor

ANS:

e.g.

energy of electron in electronic device of order meV, $10^{-3} \times 10^{-19}$J. Timescale of operation at least 10^9 Hz, more like 10^{12}Hz or higher for a modern PC. $Et \sim 10^{-31} - 10^{-34}$ or so. Maybe.

(c) bacteria swimming

ANS:

e.g.

lengthscale 10^{-6}m, so speed $\sim 10^{-6}$m/s. Density roughly that of water, so mass=$\left(10^{-6}\right)^3 = 10^{-18}$kg. $xp \sim 10^{-6} \cdot 10^{-18} \cdot 10^{-6} = 10^{-30}$. Probably not, but maybe.

(d) neurons.

ANS:

$E \sim 10$meV (action potential), $t \sim 1$ms (discharge time), $Et \sim 10^{-3} \cdot 10^{-19} \cdot 10^{-3} = 10^{-25}$ No.

1.3 The Schrödinger equation

The time dependent Schrödinger equation (TDSE) is

$$i\hbar\partial_t\psi(x,t) = \hat{H}\psi(x,t) . \tag{37}$$

1.3.1

By defining

$$\psi(x,t) = \phi(x)T(t) \tag{38}$$

show that the TDSE is separable provided the Hamiltonian $\hat{H}$ has no explicit time dependence. Derive the time independent Schrödinger equation (TISE):

$$\hat{H}\phi(x) = E\phi(x) \tag{39}$$

and solve the corresponding equation for $T(t)$.

1.3.2

For a solution to the TISE state the corresponding solution to the TDSE.

ANS:

for a solution

$$\phi(x)$$

to the TISE, the corresponding solution to the TDSE is

$$\psi(x,t) = \phi(x)\exp(-iEt/\hbar) .$$

1.3.3

A plane wave takes the form

$$\psi_L(x,t) = A_L \exp\left(i\left(-kx - \omega t\right)\right) \tag{40}$$

$$\psi_R(x,t) = A_R \exp\left(i\left(kx - \omega t\right)\right) \tag{41}$$

where L and R indicate leftgoing and rightgoing waves.

(a) Show that the Schrödinger equation returns the Einstein relation $E = \hbar\omega$.

ANS:

$$\begin{aligned} i\hbar\partial_t\psi &= E\psi \\ i\hbar\left(-i\omega\right)\psi &= E\psi \\ \hbar\omega &= E. \end{aligned}$$

(b) Show that the Schrödinger equation returns the de Broglie relation $p = \hbar k = h/\lambda$.

ANS:

$$\begin{aligned} \hat{H}\psi &= E\psi \\ -\frac{\hbar^2}{2m}\nabla^2\psi &= E\psi \\ \frac{\hbar^2k^2}{2m} &= E = \frac{p^2}{2m} \\ \hbar k &= p. \end{aligned}$$

1.3.4

If $\psi(x,t)$ describes a state evolving forwards in time, its complex conjugate $\psi(x,t)^*$ can be thought of as describing a state evolving backwards in time. Assuming a purely real Hamiltonian, explain using the TDSE why this interpretation is natural.

ANS:

$$
\begin{aligned}
i\hbar\partial_t\psi(x,t) &= \hat{H}\psi(x,t) \\
&\downarrow * \\
-i\hbar\partial_t\psi(x,t)^* &= \hat{H}\psi(x,t)^* \\
i\hbar\partial_{-t}\psi(x,t)^* &= \hat{H}\psi(x,t)^* \\
&\downarrow t \to -t \\
i\hbar\partial_t\psi(x,-t)^* &= \hat{H}\psi(x,-t)^*
\end{aligned}
$$

i.e. $\psi(x,-t)^*$ is a solution to the original TDSE with $t \to -t$.

1.4 Probability current density

1.4.1

Defining the probability density $\rho(x,t) = |\psi(x,t)|^2$ show that

$$\partial_t\rho + \partial_x j = 0 \tag{42}$$

where

$$j(x,t) = -\frac{i\hbar}{2m}\left(\psi^*\partial_x\psi - \psi\partial_x\psi^*\right). \tag{43}$$

Interpret the result physically.

1.4.2

Find $j(x,t)$ for the plane waves in Equations 40 and 41, and show that j describes the velocity of the waves.

ANS:

$$
\begin{aligned}
\psi_L &= A_L \exp\left(i\left(-kx - \omega t\right)\right) \\
j(x,t) &= -\frac{i\hbar}{2m}\left(-ik - ik\right) \\
&= -\frac{\hbar k}{m} \\
&= -p/m = v.
\end{aligned}
$$

2 Scattering and tunnelling

Bring solutions along to the class at 10am on 12/10/20.

Questions marked # are beyond the syllabus. We may discuss them in the class if there is time. Attempt all questions. Feel free to discuss with friends. Don't worry if you cannot answer a question fully as you will discuss the solutions in the class.

2.0 Videos

Please watch this week's videos: V2.1a, V2.1b, V2.1c, V2.1d, V2.2, V2.3

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

2.1 Scattering from a potential step

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

$$V(x) = \begin{cases} V_0,\ x \geq 0\,(\text{region } I) \\ 0,\ x < 0\,(\text{region } II). \end{cases} \tag{44}$$

2.1.1

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

$$\phi_I(x) = \exp(ikx) + r\exp(-ikx) \tag{45}$$

$$\phi_{II}(x) = t\exp(-\kappa x)\,. \tag{46}$$

What are the corresponding forms for $E > V_0$?

ANS:

$$\phi_{II}(x) = t\exp(ik'x)\,.$$

2.1.2

Find expressions for k and κ in terms of E and V_0, and the equivalent for $E < V_0$.

ANS:

$$k = \frac{\sqrt{2mE}}{\hbar}$$
$$\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

for $E < V_0$

$$\kappa \to -ik'.$$

2.1.3

State the two boundary conditions obeyed at the step.

ANS:

$$\phi_I(0) = \phi_{II}(0)$$
$$\phi'_I(0) = \phi'_{II}(0).$$

2.1.4

Find the reflection and transmission amplitudes for the cases

(a) $E < V_0$

ANS:

$$1 + r = t$$
$$ik(1 - r) = -\kappa t$$

therefore

$$r = \frac{k - i\kappa}{k + i\kappa}$$
$$t = \frac{2k}{k + i\kappa}.$$

(b) $E > V_0$.

ANS:

$\kappa \to -ik'$ therefore

$$r = \frac{k-k'}{k+k'}$$
$$t = \frac{2k}{k+k'}.$$

2.1.5

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

ANS:

(a)

$$R = \frac{j_R}{j_{\text{in}}} = |r|^2$$
$$T = \frac{j_T}{j_{\text{in}}} = 0.$$

(b)

$$R = \frac{j_R}{j_{\text{in}}} = |r|^2$$
$$T = \frac{j_T}{j_{\text{in}}} = \frac{k'}{k}|t|^2 = \sqrt{1 - \frac{V_0}{E}}\,|t|^2\,.$$

2.1.6

Show that $R + T = 1$ in both cases.

2.1.7

Show that if the step occurs at $x = a$ instead of $x = 0$ the reflection and transmission amplitudes change, but the reflection and transmission probabilities remain the same.

ANS:

$$V(x) = \begin{cases} V_0,\ x \geq a\,(\text{region } 1) \\ 0,\ x < a\,(\text{region } 2). \end{cases}$$

For $E < V_0$ we still have a real ϕ_{II} and so $j_T = 0$ and $T = 0$. Therefore $R = 1$.

For $E > V_0$

$$\phi_I(a) = \phi_{II}(a)$$
$$\phi'_I(a) = \phi'_{II}(a).$$

$$(i):\ \exp(ika) + r\exp(-ika) = t\exp(ik'a)$$
$$(ii):\ \exp(ika) - r\exp(-ika) = \frac{k'}{k} t\exp(ik'a)$$

$$(i)+(ii):\ 2\exp(ika) = t\exp(ik'a)\left(1 + \frac{k'}{k}\right)$$
$$t = \exp(i(k-k')a)\frac{2k}{k+k'}$$

$$(i)-(ii):\ 2r\exp(-ika) = t\exp(ik'a)\left(1 - \frac{k'}{k}\right)$$
$$r = \frac{2k}{k+k'}\exp(2ika)$$

both only change by a phase from the $a = 0$ case, so T and R unchanged.

2.1.8

Sketch the waves in each region, paying attention to the amplitude, phase, and wavelength of the waves, for the following cases:

(a) $E \gg V_0$

ANS:

$$\frac{k'}{k} = \sqrt{1 - \frac{V_0}{E}}$$
$$\approx 1 - \frac{V_0}{2E}$$

$$r \approx \frac{V_0}{4E} \approx 0$$
$$t \approx \frac{4E}{4E - V_0} \approx 1.$$

(b) $E \gtrsim V_0$

ANS:

$$\frac{k'}{k} = \sqrt{1 - \frac{V_0}{E}}$$

let $V_0/E \triangleq 1 - \epsilon^2$

$$\frac{k'}{k} = \epsilon$$
$$\lambda = \epsilon \lambda'$$

$$r = \frac{1-\epsilon}{1+\epsilon} \approx 1$$
$$t = \frac{2}{1+\epsilon} \approx 2$$

but note that $|r|^2 + |t|^2 (k'/k)^2 = 1$ as required.

(c) $E \lesssim V_0$

ANS:

$$\frac{\kappa}{k} = \sqrt{\frac{V_0}{E} - 1} \triangleq \epsilon \to 0$$

$$\kappa = \frac{2\pi\epsilon}{\lambda} : \text{ slow decay compared to } \lambda$$

$$t = 2\left(1 - i\epsilon\right) \approx 2$$
$$r = \frac{1 - i\epsilon}{1 + i\epsilon} \approx 1$$

(d) $E \approx 0$.

ANS:

$$\frac{\kappa}{k} \to \infty$$
$$t \to 0$$
$$r \to -1 : \pi \text{ phase shift}$$

2.1.9

Derive the transmission and reflection amplitudes and probabilities assuming instead the potential

$$V\left(x\right) = \begin{cases} V_0, \; x < 0 \,(\text{region } 1) \\ 0, \; x \geq 0 \,(\text{region } 2) \end{cases} \tag{47}$$

but with the wave still incident from the left ($x = -\infty$). Explain why we require $E > V_0$ in this case.

2.2 Scattering over a barrier

Consider the potential

$$V(x) = \begin{cases} 0,\ x < -L\,(\text{region 1}) \\ V_0,\ -L \le x \le L\,(\text{region 2}) \\ 0,\ x \ge L\,(\text{region 3}). \end{cases} \tag{48}$$

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

$$\phi_1 = \exp(ikx) + r\exp(-ikx) \tag{49}$$

$$\phi_2 = a\exp(ik'x) + b\exp(-ik'x) \tag{50}$$

$$\phi_3 = t\exp(-ikx)\,. \tag{51}$$

2.2.1

Sketch the potential.

2.2.2

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

ANS:

$$k = \frac{\sqrt{2mE}}{\hbar}$$

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

2.2.3

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

ANS:

$$\phi_1(-L) = \phi_2(-L)$$

$$\phi_1'(-L) = \phi_2'(-L)$$

$$\phi_2(L) = \phi_3(L)$$

$$\phi_2'(L) = \phi_3'(L)$$

2.2.4

(a) Show that the four boundary conditions lead to the matrix equation

$$\begin{pmatrix} -\exp(ikL) & \exp(-ik'L) & \exp(ik'L) & 0 \\ k\exp(ikL) & k'\exp(-ik'L) & -k'\exp(ik'L) & 0 \\ 0 & \exp(ik'L) & \exp(-ik'L) & -\exp(ikL) \\ 0 & k'\exp(ik'L) & -k'\exp(-ik'L) & -k\exp(ikL) \end{pmatrix} \begin{pmatrix} r \\ a \\ b \\ t \end{pmatrix} = \begin{pmatrix} \exp(-ikL) \\ k\exp(-ikL) \\ 0 \\ 0 \end{pmatrix}. \quad (52)$$

(b) Calling the matrix M, show that

$$t = \exp(-ikL)\left(M^{-1}_{41} + kM^{-1}_{42}\right) = \frac{\exp(-ikL)}{\det(M)}\left(C^{-1}_{14} + kC^{-1}_{24}\right) \quad (53)$$

where C is the matrix of signed cofactors.

ANS:

This follows from acting the inverse matrix from the left.

2.2.5

The resonant transmission condition is that $k'L = n\pi$ for integer n.

(a) For which energies is the barrier at resonance?

ANS:

$$E = V_0 + \frac{\hbar^2 k'^2}{2m} = V_0 + \frac{h^2 n^2}{8mL^2}.$$

(b) Considering the case of n even, show that Eqn. 52 can be written

$$\begin{pmatrix} -1 & 1 & 1 & 0 \\ k & k' & -k' & 0 \\ 0 & 1 & 1 & -1 \\ 0 & k' & -k' & -k \end{pmatrix} \begin{pmatrix} r\exp(ikL) \\ a \\ b \\ t\exp(ikL) \end{pmatrix} = \begin{pmatrix} \exp(-ikL) \\ k\exp(-ikL) \\ 0 \\ 0 \end{pmatrix}. \quad (54)$$

(c) Therefore, using the rules for simplifying determinants, show that the probability of transmission is indeed one, and that of reflection is zero.

ANS:

$$\begin{aligned}
\det(M) &= \begin{vmatrix} -1 & 1 & 1 & 0 \\ k & k' & -k' & 0 \\ 0 & 1 & 1 & -1 \\ 0 & k' & -k' & -k \end{vmatrix} \\
&= \begin{vmatrix} -1 & 2 & 1 & 0 \\ k & 0 & -k' & 0 \\ 0 & 2 & 1 & -1 \\ 0 & 0 & -k' & -k \end{vmatrix} \\
&= -\begin{vmatrix} 0 & -k' & 0 \\ 2 & 1 & -1 \\ 0 & -k' & -k \end{vmatrix} - 2k \begin{vmatrix} 1 & 0 & 0 \\ 1 & 0 & -1 \\ 0 & -k' & -k \end{vmatrix} \\
&= 2kk' - 2k\left(k'\right) \\
&= 4kk'
\end{aligned}$$

$$\begin{aligned}
C_{14}^{-1} &= -\begin{vmatrix} k & k' & -k' \\ 0 & 1 & 1 \\ 0 & k' & -k' \end{vmatrix} \\
&= -\begin{vmatrix} k & 0 & 0 \\ 0 & 1 & 1 \\ 0 & k' & -k' \end{vmatrix} \\
&= 2kk'
\end{aligned}$$

$$\begin{aligned}
C_{24}^{-1} &= \begin{vmatrix} -1 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & k' & -k' \end{vmatrix} \\
&= \begin{vmatrix} -1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & k' & -k' \end{vmatrix} \\
&= 2k'
\end{aligned}$$

Therefore

$$t \exp(ikL) = \frac{2kk' \exp(-ikL) + 2k'k \exp(-ikL)}{4kk'}$$
$$t = \exp(-2ikL)$$
$$T = |t|^2 = 1.$$

You can do the same for r, or argue that $R + T = 1$.

2.2.6 Scattering over a finite potential well

Switching the sign of V_0 in Eq. 48 gives the potential of a finite well. Later in the course we will see that this is able to trap bound states for $E < 0$. However, if $E > 0$ the solutions are still plane waves. For what values of the energy will a plane wave pass unhindered through the well?

ANS:

$$V_0 \to -V_0$$

and so the resonance condition is

$$E = \frac{h^2 n^2}{8mL^2} - V_0.$$

2.3 Quantum tunnelling

Return to the potential of Eq. 48 in 2.2. Now consider the case $E < V_0$.

2.3.1

What are the classical probabilities for transmission and reflection?

ANS:
0 and 1, respectively.

2.3.2

Explain why the only change to the form of the wavefunctions is to change $k' \to -i\kappa$ in Eq. 50.

ANS:
Same equation, but evanescent waves expected in classically forbidden region. Substitution ensures κ real.

2.3.3

Identify the condition on κ in terms of E and V_0.

ANS:

$$\kappa = \frac{\sqrt{2m\left(V_0 - E\right)}}{\hbar.}$$

2.3.4

Deduce that the matrix equation, Eq. 52, changes to

$$\begin{pmatrix} -\exp\left(ikL\right) & \exp\left(-\kappa L\right) & \exp\left(\kappa L\right) & 0 \\ k\exp\left(ikL\right) & -i\kappa\exp\left(-\kappa L\right) & i\kappa\exp\left(\kappa L\right) & 0 \\ 0 & \exp\left(\kappa L\right) & \exp\left(-\kappa L\right) & -\exp\left(ikL\right) \\ 0 & -i\kappa\exp\left(\kappa L\right) & i\kappa\exp\left(-\kappa L\right) & -k\exp\left(ikL\right) \end{pmatrix} \begin{pmatrix} r \\ a \\ b \\ t \end{pmatrix} = \begin{pmatrix} \exp\left(-ikL\right) \\ k\exp\left(-ikL\right) \\ 0 \\ 0 \end{pmatrix}. \tag{55}$$

2.3.5

Is resonant transmission possible?

ANS:

No, as $\exp\left(\pm\kappa L\right) \neq 1$ for $\kappa > 0$.

2.3.6

Show that the probability of transmission through the barrier is

$$T = \frac{4k^2\kappa^2}{4k^2\kappa^2 + \left(\kappa^2 + k^2\right)^2 \sinh^2\left(2\kappa L\right)}. \tag{56}$$

HINT: use Eq. 53 and the rules for simplifying determinants.

ANS:

$$t = \frac{\exp\left(-ikL\right)}{\det\left(M\right)}\left(C_{14}^{-1} + kC_{24}^{-1}\right)$$

$$C_{14}^{-1} = -\begin{vmatrix} k\exp\left(ikL\right) & -i\kappa\exp\left(-\kappa L\right) & i\kappa\exp\left(\kappa L\right) \\ 0 & \exp\left(\kappa L\right) & \exp\left(-\kappa L\right) \\ 0 & -i\kappa\exp\left(\kappa L\right) & i\kappa\exp\left(-\kappa L\right) \end{vmatrix} = -k\exp\left(ikL\right)\begin{vmatrix} \exp\left(\kappa L\right) & \exp\left(-\kappa L\right) \\ -i\kappa\exp\left(\kappa L\right) & i\kappa\exp\left(-\kappa L\right) \end{vmatrix}$$

$$= -2i\kappa k\exp\left(ikL\right)$$

$$C_{24}^{-1} = \begin{vmatrix} -\exp(ikL) & \exp(-\kappa L) & \exp(\kappa L) \\ 0 & \exp(\kappa L) & \exp(-\kappa L) \\ 0 & -i\kappa \exp(\kappa L) & i\kappa \exp(-\kappa L) \end{vmatrix}$$
$$= -2i\kappa \exp(ikL)$$

Therefore

$$t = \frac{-4ik\kappa}{\det(M)}$$

and

$$\det(M) = \begin{vmatrix} -\exp(ikL) & \exp(-\kappa L) & \exp(\kappa L) & 0 \\ k\exp(ikL) & -i\kappa\exp(-\kappa L) & i\kappa\exp(\kappa L) & 0 \\ 0 & \exp(\kappa L) & \exp(-\kappa L) & -\exp(ikL) \\ 0 & -i\kappa\exp(\kappa L) & i\kappa\exp(-\kappa L) & -k\exp(ikL) \end{vmatrix}$$

$$= -\exp(ikL)\begin{vmatrix} -i\kappa\exp(-\kappa L) & i\kappa\exp(\kappa L) & 0 \\ \exp(\kappa L) & \exp(-\kappa L) & -\exp(ikL) \\ -i\kappa\exp(\kappa L) & i\kappa\exp(-\kappa L) & -k\exp(ikL) \end{vmatrix}$$

$$-k\exp(ikL)\begin{vmatrix} \exp(-\kappa L) & \exp(\kappa L) & 0 \\ \exp(\kappa L) & \exp(-\kappa L) & -\exp(ikL) \\ -i\kappa\exp(\kappa L) & i\kappa\exp(-\kappa L) & -k\exp(ikL) \end{vmatrix}$$

$$= -\exp(ikL)\begin{vmatrix} -i\kappa\exp(-\kappa L) & i\kappa\exp(\kappa L) & 0 \\ \exp(\kappa L) & \exp(-\kappa L) & -\exp(ikL) \\ 0 & 2i\kappa\exp(-\kappa L) & -(k+i\kappa)\exp(ikL) \end{vmatrix}$$

$$-k\exp(ikL)\begin{vmatrix} \exp(-\kappa L) & \exp(\kappa L) & 0 \\ \exp(\kappa L) & \exp(-\kappa L) & -\exp(ikL) \\ 0 & 2i\kappa\exp(-\kappa L) & -(k+i\kappa)\exp(ikL) \end{vmatrix}$$

$$-\det(M)\exp(-ikL) = -i\kappa\exp(-\kappa L)\begin{vmatrix} \exp(-\kappa L) & -\exp(ikL) \\ 2i\kappa\exp(-\kappa L) & -(k+i\kappa)\exp(ikL) \end{vmatrix}$$

$$-\exp(\kappa L)\begin{vmatrix} i\kappa\exp(\kappa L) & 0 \\ 2i\kappa\exp(-\kappa L) & -(k+i\kappa)\exp(ikL) \end{vmatrix}$$

$$+k\exp(-\kappa L)\begin{vmatrix} \exp(-\kappa L) & -\exp(ikL) \\ 2i\kappa\exp(-\kappa L) & -(k+i\kappa)\exp(ikL) \end{vmatrix}$$

$$-k\exp(\kappa L)\begin{vmatrix} \exp(\kappa L) & 0 \\ 2i\kappa\exp(-\kappa L) & -(k+i\kappa)\exp(ikL) \end{vmatrix}$$

$$= [-i\kappa(-k+i\kappa) + k(-k+i\kappa)]\exp((ik-2\kappa)L) + [i\kappa(k+i\kappa) + k(k+i\kappa)]\exp((ik+2\kappa)L)$$

$$= \left[2i\kappa k + \kappa^2 - k^2\right]\exp((ik-2\kappa)L) + \left[2i\kappa k - \kappa^2 + k^2\right]\exp((ik+2\kappa)L)$$

$$\det(M)\exp(-2ikL) = -4i\kappa k\cosh(2\kappa L) + 2\left[\kappa^2 - k^2\right]\sinh(2\kappa L)$$

Therefore

$$t = \frac{-4ik\kappa}{-4i\kappa k\cosh(2\kappa L) + 2\left[\kappa^2 - k^2\right]\sinh(2\kappa L)}\exp(-2ikL)$$

$$= \frac{4k\kappa}{4\kappa k\cosh(2\kappa L) + 2i\left[\kappa^2 - k^2\right]\sinh(2\kappa L)}\exp(-2ikL)$$

and

$$\begin{aligned}T = \frac{j_T}{j_{in}} = |t|^2 &= \frac{(4k\kappa)^2}{(4\kappa k)^2 \cosh^2(2\kappa L) + 4\left[\kappa^2 - k^2\right]^2 \sinh^2(2\kappa L)} \\ &= \frac{4k^2\kappa^2}{4k^2\kappa^2 + (\kappa^2 + k^2)^2 \sinh^2(2\kappa L)}.\end{aligned}$$

2.3.7

Hence show that

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

Does this make sense with regard to the barrier penetration problem shown in the notes and lectures?

ANS: yes, the barrier length is $2L$ here.

3 Bound states (I)

Bring solutions along to the class at 10am on 19/10/20.

Questions marked # are beyond the syllabus. We may discuss them in the class if there is time.

Attempt all questions. Feel free to discuss with friends. Don't worry if you cannot answer a question fully as you will discuss the solutions in the class.

3.0 Videos

Please watch this week's videos: V3.1, V3.2, V3.3, V3.4, V3.5

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

3.1 The infinite potential well

Consider the TISE

$$\left(-\frac{\hbar^2}{2m}\partial_x^2 + V(x)\right)\phi_n(x) = E_n\phi_n(x) \tag{57}$$

with the potential

$$V(x) = \begin{cases} 0, & -L/2 \le x \le L/2 \\ \infty, & \text{otherwise.} \end{cases} \tag{58}$$

3.1.1

Sketch the potential and the first five energy eigenfunctions.

3.1.2

Which eigenfunctions $\phi_n(x)$ will be odd, and which even? Bearing this in mind will help simplify many of the remaining questions!

ANS: ϕ_n odd for n even, even for n odd.

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

ANS:

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

The global phase is unobservable.

3.1.4

Show that all eigenfunctions are orthonormal.

ANS: odd×even cases automatically zero.

$$\frac{2}{L}\int_{-L/2}^{L/2}\cos\left(\frac{n\pi x}{L}\right)\cos\left(\frac{m\pi x}{L}\right)\mathrm{d}x = \frac{1}{L}\int_{-L/2}^{L/2}\left(\cos\left(\frac{(n+m)\,\pi x}{L}\right)+\cos\left(\frac{(n-m)\,\pi x}{L}\right)\right)\mathrm{d}x$$
$$= \frac{2}{\pi}\left[\frac{1}{n+m}\sin\left(\frac{(n+m)\,\pi}{2}\right)+\frac{1}{n-m}\sin\left(\frac{(n-m)\,\pi}{2}\right)\right]$$

for $n \neq m$ this is zero as n, m both odd, and $\sin\left((\text{even})\,\pi/2\right) = 0$. For $n = m$ it is one, as l'Hôpital's rule on the second term.

3.1.5

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

$$\psi_n(x,t) = \begin{cases} \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right)\exp\left(-\frac{i\hbar n^2\pi^2 t}{2mL^2}\right), & n \text{ odd} \\ \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)\exp\left(-\frac{i\hbar n^2\pi^2 t}{2mL^2}\right), & n \text{ even} \end{cases}$$

3.1.6

Show that the probability density

$$\rho(x) = \left|\psi_n(x,t)\right|^2 \tag{59}$$

is time independent for all energy eigenfunctions.

ANS:

In general, time dependence is a complex phase. QED.

3.1.7

Say the particle in the well is known to have energy E_3. What is the probability to find the particle in the leftmost quarter of the well?

ANS:

$$
\begin{aligned}
P\left(-\frac{L}{2} \le x \le -\frac{L}{4}\right) &= \int_{-L/2}^{-L/4} |\psi_3|^2 \,\mathrm{d}x \\
&= \frac{2}{L}\int_{-L/2}^{-L/4} \cos^2\left(\frac{3\pi x}{L}\right)\mathrm{d}x \\
&= \frac{1}{L}\int_{-L/2}^{-L/4} \left(1+\cos\left(\frac{6\pi x}{L}\right)\right)\mathrm{d}x \\
&= \frac{1}{L}\left[x + \frac{L}{6\pi}\sin\left(\frac{6\pi x}{L}\right)\right]_{-L/2}^{-L/4} \\
&= \frac{1}{L}\left[\frac{L}{4} - \frac{L}{6\pi}\sin\left(\frac{3\pi}{2}\right) + \frac{L}{2n\pi}\sin\left(3\pi\right)\right] \\
&= \frac{1}{4} + \frac{1}{6\pi}.
\end{aligned}
$$

3.1.8

Explain, without detailed calculation, why the expectation values of position, defined as:

$$\langle\hat{x}\rangle \triangleq \int_{-\infty}^{\infty} \psi_n^*(x,t)\, x\psi_n(x,t)\,\mathrm{d}x \tag{60}$$

and momentum, defined as:

$$\langle\hat{p}\rangle \triangleq \int_{-\infty}^{\infty} \psi_n^*(x,t)\left(-i\hbar\partial_x\right)\psi_n(x,t)\,\mathrm{d}x \tag{61}$$

must be zero for any energy eigenfunction in the well.

ANS: odd×even.

3.1.9

At which positions are you most likely to find a particle described by eigenstate ψ_n? Explain why there is no contradition with the previous result.

ANS:

$$-\frac{L}{2} + \frac{Lp}{n+1},\ p < n.$$

By inspection, or $\partial_x \rho_n(x) = 0$. No contradiction as expectation value is not the most probable place to find the particle.

3.1.10

(a) The expected value of x^2 for eigenstate ψ_n is

$$\langle \hat{x}^2 \rangle = \int_{-\infty}^{\infty} \psi_n^* (x,t) \, x^2 \psi_n (x,t) \, \mathrm{d}x. \tag{62}$$

Show that

$$\langle \hat{x}^2 \rangle = \frac{L^2}{12} + \frac{L^2}{2n^2\pi^2}. \tag{63}$$

ANS:

$$\begin{aligned}
\int \psi_n^* (x,t) \, x^2 \psi_n (x,t) \, \mathrm{d}x &= \frac{2}{L} \int_{-L/2}^{L/2} x^2 \left\{ \begin{array}{l} \cos^2\left(\frac{n\pi x}{L}\right), \, n \text{ odd} \\ \sin^2\left(\frac{n\pi x}{L}\right), \, n \text{ even} \end{array} \right\} \mathrm{d}x \\
&= \frac{1}{L} \int_{-L/2}^{L/2} x^2 \mathrm{d}x - (-1)^n \frac{1}{L} \int_{-L/2}^{L/2} x^2 \cos\left(\frac{2n\pi x}{L}\right) \mathrm{d}x \\
&= \frac{L^2}{12} - \frac{(-1)^n}{L} \left\{ \left[\frac{L}{2\pi n} x^2 \sin\left(\frac{2n\pi x}{L}\right) \right]_{-L/2}^{L/2} - \frac{L}{n\pi} \int_{-L/2}^{L/2} x \sin\left(\frac{2n\pi x}{L}\right) \mathrm{d}x \right\} \\
&= \frac{L^2}{12} - \frac{(-1)^n}{L} \left\{ -\frac{L^3}{2n^2\pi^2} \cos(n\pi) + \frac{L^3}{4n^3\pi^3} \left[\sin\left(\frac{2n\pi x}{L}\right) \right]_{-L/2}^{L/2} \right\} \\
&= \frac{L^2}{12} + \frac{L^2}{2n^2\pi^2}
\end{aligned}$$

(b) The expected value of p^2 for eigenstate ψ_n is

$$\langle \hat{p}^2 \rangle = \int_{-\infty}^{\infty} \psi_n^* (x,t) \left(-i\hbar\partial_x\right)^2 \psi_n (x,t) \, \mathrm{d}x. \tag{64}$$

Show that

$$\langle \hat{p}^2 \rangle = \left(\frac{\hbar n \pi}{L} \right)^2. \tag{65}$$

HINT: one method is to use the TISE.

ANS:

$$\begin{aligned}
\int \psi_n^* (x,t) \, \hat{p}^2 \psi_n (x,t) \, \mathrm{d}x &= 2m \int \psi_n^* (x,t) \, \hat{H} \psi_n (x,t) \, \mathrm{d}x \\
&= 2m \int \psi_n^* (x,t) \, E_n \psi_n (x,t) \, \mathrm{d}x \\
&= 2mE_n.
\end{aligned}$$

(c) The Heisenberg uncertainty principle states that

$$\sigma_x \sigma_p \geq \frac{\hbar}{2} \tag{66}$$

where

$$\sigma_{\hat{A}} \triangleq \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2} \tag{67}$$

is the uncertainty (standard deviation). Show that the uncertainty principle is obeyed by the eigenstates of the infinite well.

ANS:

$$\begin{aligned}\sigma_x \sigma_p &= \sqrt{\langle \hat{x}^2 \rangle}\sqrt{\langle \hat{p}^2 \rangle} \\ &= \frac{\hbar}{2}\sqrt{2 + \frac{n^2\pi^2}{3}} > \frac{\hbar}{2}.\end{aligned}$$

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:

$$\int_{-\infty}^{\infty} \phi_n^*(x)\,\phi_m(x)\,\mathrm{d}x = \delta_{nm} \tag{68}$$

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

$$f(x) = \sum_{n=1}^{\infty} f_n \phi_n(x) \tag{69}$$

and identify the (possibly complex) coefficients f_n.

ANS:

$$\begin{aligned}\int_{-\infty}^{\infty} \phi_m^*(x)\, f(x)\,\mathrm{d}x &= \sum_{n=1}^{\infty} f_n \int_{-\infty}^{\infty} \phi_m^*(x)\,\phi_n(x)\,\mathrm{d}x \\ &= \sum_{n=1}^{\infty} f_n \delta_{nm} \\ &= f_m.\end{aligned}$$

4 Bound states (II)

Bring solutions along to the class at 10am on 26/11/20.

Questions marked # are beyond the syllabus. We may discuss them in the class if there is time. Attempt all questions. Feel free to discuss with friends. Don't worry if you cannot answer a question fully as you will discuss the solutions in the class.

4.0 Videos

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4.1 Linearity of quantum mechanics

Show that if

$$\psi_n(x,t) = \phi_n(x) \exp(-iE_n t/\hbar) \tag{70}$$

is a solution to the TDSE, then any superposition

$$f(x,t) = \sum_{n=1}^{\infty} f_n \psi_n(x,t) \tag{71}$$

is also a solution.

ANS:

we need to show that

$$i\hbar\partial_t f(x,t) = \hat{H} f(x,t)$$

given

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

Act $i\hbar\partial_t$ on Eq. 71:

$$\begin{aligned} i\hbar\partial_t f(x,t) &= \sum_{n=1}^{\infty} f_n i\hbar\partial_t \psi_n(x,t) \\ &= \sum_{n=1}^{\infty} f_n \hat{H}\psi_n(x,t) \\ &= \hat{H}\sum_{n=1}^{\infty} f_n \psi_n(x,t) \end{aligned}$$

QED.

4.2 Superposition of two energy eigenstates

Consider again the infinite well potential of Eq. 58, and the energy eigenvalues and normalized eigenvectors you found in question **3.1.3**.

4.2.1

Consider the state

$$\chi(x,t) = \mathcal{N}\left(3\psi_1(x,t) + 4\psi_2(x,t)\right). \tag{72}$$

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

ANS: 1/5.

4.2.2

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

ANS:

E_1 and E_2.

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

ANS:

$P_1 = 9/25,\ P_2 = 16/25,\ P_{n>2} = 0.$

4.2.3

Find the time-dependent probability density of $\chi(x,t)$. After how long does the state return to its original form?

ANS:

$$\begin{aligned}|\chi(x,t)|^2 &= \frac{1}{25}\left(9|\psi_1(x,t)|^2 + 16|\psi_2(x,t)|^2 + 24\phi_1(x)\phi_2(x)\cos((E_2-E_1)t/\hbar)\right)\\ &= \frac{2}{25L}\left(9\cos^2\left(\frac{\pi x}{L}\right) + 16\sin^2\left(\frac{2\pi x}{L}\right) + 24\cos\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{3\hbar\pi^2 t}{2mL^2}\right)\right)\end{aligned}$$

Returns to itself when

$$\begin{aligned}\frac{3\hbar\pi^2 T}{2mL^2} &= 2\pi\\ T &= \frac{8mL^2}{3h}.\end{aligned}$$

4.2.4

Show that the expected value of position for the state $\chi(x,t)$ is

$$\langle x\rangle_\chi = \left(\frac{L}{2}\right)\cdot\frac{2^8}{75\pi^2}\cos\left(\frac{3\hbar\pi^2 t}{2mL^2}\right).$$

HINT:

$$\begin{aligned}\cos(Ax)\sin(2Ax) &= 2\cos^2(Ax)\sin(Ax) &(73)\\ &= -\frac{2}{3A}\frac{\mathrm{d}}{\mathrm{d}x}\left(\cos^3(Ax)\right) &(74)\\ &= -\frac{1}{6A}\frac{\mathrm{d}}{\mathrm{d}x}\left(\cos(3Ax)+3\cos(Ax)\right) &(75)\end{aligned}$$

(check you can derive each step!).

ANS:

$$\langle\chi|x|\chi\rangle = \frac{2}{25L}\int_{-L/2}^{L/2} x\left(9\cos^2\left(\frac{\pi x}{L}\right)+16\sin^2\left(\frac{2\pi x}{L}\right)+24\cos\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{3\hbar\pi^2 t}{2mL^2}\right)\right)\mathrm{d}x$$

$$\begin{aligned}
&\downarrow \text{odd}\times\text{even}\\
&= \frac{48}{25L}\cos\left(\frac{3\hbar\pi^2 t}{2mL^2}\right)\int_{-L/2}^{L/2} x\cos\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)\mathrm{d}x\\
&= -\frac{32}{25\pi}\cos\left(\frac{3\hbar\pi^2 t}{2mL^2}\right)\int_{-L/2}^{L/2} x\frac{\mathrm{d}}{\mathrm{d}x}\left(\cos^3\left(\frac{\pi x}{L}\right)\right)\mathrm{d}x\\
&= -\frac{32}{25\pi}\cos\left(\frac{3\hbar\pi^2 t}{2mL^2}\right)\left\{\left[x\cos^3\left(\frac{\pi x}{L}\right)\right]_{-L/2}^{L/2} - \int_{-L/2}^{L/2}\cos^3\left(\frac{\pi x}{L}\right)\mathrm{d}x\right\}\\
&= \frac{8}{25\pi}\cos\left(\frac{3\hbar\pi^2 t}{2mL^2}\right)\int_{-L/2}^{L/2}\left(\cos\left(\frac{3\pi x}{L}\right)+3\cos\left(\frac{\pi x}{L}\right)\right)\mathrm{d}x\\
&= \frac{2^7 L}{75\pi^2}\cos\left(\frac{3\hbar\pi^2 t}{2mL^2}\right)\\
&\approx 0.34\cos\left(\frac{3\hbar\pi^2 t}{2mL^2}\right)\left(\frac{L}{2}\right).
\end{aligned}$$

4.3 Deriving the time evolution of a given state

Consider again the infinite well potential of Eq. 58, and the energy eigenvalues and normalized eigenvectors you found in question **3.1.3**. A state is prepared in the well which has a wavefunction given by a top hat function:

$$\varpi(x) = \begin{cases} (\alpha L)^{-1/2},\ -\alpha\frac{L}{2} \le x \le \alpha\frac{L}{2} \\ 0,\ \text{otherwise} \end{cases} \tag{76}$$

where $0 < \alpha \le 1$.

4.3.1

Check this state is normalised.

4.3.2

Show that this state can be written in terms of energy eigenstates as:

$$\varpi(x) = \sqrt{2\alpha}\sum_{n\ \text{odd}} \text{sinc}\left(\frac{n\pi\alpha}{2}\right)\phi_n(x). \tag{77}$$

ANS:

$$\begin{aligned}\varpi(x) &= \sum_n \left(\int_{-\infty}^{\infty} \phi_n^*(x)\,\varpi(x)\,\mathrm{d}x\right)\phi_n(x)\\ &= \sum_n \left((\alpha L)^{-1/2}\int_{-\alpha L/2}^{\alpha L/2} \phi_n^*(x)\,\mathrm{d}x\right)\phi_n(x)\end{aligned}$$

even n:

$$\sqrt{\frac{2}{\alpha}}\frac{1}{L}\int_{-\alpha L/2}^{\alpha L/2} \sin\left(\frac{n\pi x}{L}\right)\mathrm{d}x = 0.$$

Odd n:

$$\sqrt{\frac{2}{\alpha}}\frac{1}{L}\int_{-\alpha L/2}^{\alpha L/2} \cos\left(\frac{n\pi x}{L}\right)\mathrm{d}x = \sqrt{\frac{2}{\alpha}}\frac{2}{n\pi}\sin\left(\frac{n\pi\alpha}{2}\right)$$

therefore

$$\begin{aligned}\varpi(x) &= \sqrt{\frac{2}{\alpha}}\sum_{n\text{ odd}} \frac{2\sin\left(\frac{n\pi\alpha}{2}\right)}{n\pi}\phi_n(x)\\ &= \sqrt{2\alpha}\sum_{n\text{ odd}} \frac{2\sin\left(\frac{n\pi\alpha}{2}\right)}{n\pi\alpha}\phi_n(x)\end{aligned}$$

4.3.3

State the subsequent time evolution.

ANS:

$$\varpi(x,t) = \sqrt{2\alpha}\sum_{n\text{ odd}} \operatorname{sinc}\left(\frac{n\pi\alpha}{2}\right)\psi_n(x,t)\,.$$

4.3.4

Using the known result

$$\sum_{n\text{ odd}}^{\infty} \operatorname{sinc}^2(n) = \frac{\pi}{4} \tag{78}$$

show explicitly that $\varpi(x)$ in Eq. 77 is normalised for the case $\alpha = 2/\pi$.

ANS:

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

'explicitly' here means to use the referenced form rather than the general case:

$$\begin{aligned}
1 &= \int_{-L/2}^{L/2} \left| \sqrt{2\alpha} \sum_{n \text{ odd}} \mathrm{sinc}\left(\frac{n\pi\alpha}{2}\right) \phi_n(x) \right|^2 \mathrm{d}x \\
&= 2\alpha \sum_{n \text{ odd}} \sum_{m \text{ odd}} \mathrm{sinc}\left(\frac{n\pi\alpha}{2}\right) \mathrm{sinc}\left(\frac{m\pi\alpha}{2}\right) \int_{-L/2}^{L/2} \phi_n^*(x) \phi_m(x) \, \mathrm{d}x \\
&= 2\alpha \sum_{n \text{ odd}} \sum_{m \text{ odd}} \mathrm{sinc}\left(\frac{n\pi\alpha}{2}\right) \mathrm{sinc}\left(\frac{m\pi\alpha}{2}\right) \delta_{nm} \\
&= 2\alpha \sum_{n \text{ odd}} \mathrm{sinc}^2\left(\frac{n\pi\alpha}{2}\right)
\end{aligned}$$

then use $\alpha = 2/\pi$:

$$1 = \frac{4}{\pi} \sum_{n \text{ odd}} \mathrm{sinc}^2(n)$$

QED.

4.3.5

Given that we already know the state must be normalised, derive an expression for

$$\sum_{n \text{ odd}}^{\infty} \mathrm{sinc}^2(\beta n) \tag{79}$$

for arbitrary real β.

ANS:

from the last part we have

$$1 = 2\alpha \sum_{n\ \mathrm{odd}} \mathrm{sinc}^2\left(\frac{n\pi\alpha}{2}\right)$$

so call $\beta \triangleq \pi\alpha/2$:

$$1 = \frac{4\beta}{\pi} \sum_{n\ \mathrm{odd}} \mathrm{sinc}^2(\beta n)$$

giving

$$\sum_{n\ \mathrm{odd}}^{\infty} \mathrm{sinc}^2(\beta n) = \frac{\pi}{4\beta}.$$

4.3.6

By considering the limit $\alpha \to 0$, explain why an observation of the particle at the centre of the well implies the particle is equally likely to be observed in the left half of the well as the right for all subseqent times.

4.4 The finite potential well

Consider the potential

$$V(x) = \begin{cases} 0,\ x \leq -L & \text{(region 1)} \\ -V_0,\ -L < x < L & \text{(region 2)} \\ 0,\ L \leq x & \text{(region 3)} \end{cases} \tag{80}$$

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

4.4.1

Sketch the potential and three bound states, assuming three exist.

4.4.2

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

ANS:

$$\phi_1(-L) = \phi_2(-L)$$
$$\phi_1'(-L) = \phi_2'(-L)$$
$$\phi_2(L) = \phi_3(L)$$
$$\phi_2'(L) = \phi_3'(L)$$

4.4.3

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

$$\phi_1(x) = A\exp(\kappa x) \tag{81}$$
$$\phi_2(x) = B\cos(kx) + C\sin(kx) \tag{82}$$
$$\phi_3(x) = D\exp(-\kappa x). \tag{83}$$

Find expressions for κ and k as functions of energy.

ANS:

$$-\frac{\hbar^2\kappa^2}{2m} = E$$
$$\frac{\hbar^2 k^2}{2m} = E + V_0.$$

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

ANS:

the potentials in regions 1 and 3 are identical so by symmetry κ is the same.

(c) Why must the wavefunction be symmetric or antisymmetric? State the constraints on the coefficients in each case.

ANS:

Symmetric: $A = D$, $C = 0$. Antisymmetric: $A = -D$, $B = 0$.

(d) Use the boundary conditions to find constraints on k and κ

symmetric:

$$A \exp(-\kappa L) = B \cos(kL)$$
$$\kappa A \exp(-\kappa L) = kB \sin(kL)$$
$$\downarrow$$
$$\kappa = k \tan(kL)$$

antisymmetric:

$$A \exp(-\kappa L) = -C \sin(kL)$$
$$\kappa A \exp(-\kappa L) = kC \cos(kL)$$
$$\downarrow$$
$$\kappa = -k \cot(kL)\,.$$

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

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

ANS:

It must be symmetric (by appeal to the infinite well).

$$\kappa = k \tan(kL)$$
$$\downarrow$$
$$-E = (E + V_0) \tan^2\left(\frac{\sqrt{2m(E+V_0)}}{\hbar} L\right)$$

if V_0 is small then E is even smaller. Expand the $\tan^2$:

$$-E = \frac{2m(E+V_0)^2}{\hbar^2} L^2$$
$$0 = E^2 + E\left(2V_0 + \frac{\hbar^2}{2mL^2}\right) + V_0^2$$
$$-E = V_0 + \frac{\hbar^2}{4mL^2}\left(1 \pm \sqrt{1 + \frac{8V_0 mL^2}{\hbar^2}}\right)$$

4.4.4

Why can the unbound states not be normalized?

5 Finite-dimensional Hilbert spaces

Bring solutions along to the class at 10am on 2/11/20.

Questions marked # are beyond the syllabus. We may discuss them in the class if there is time. Attempt all questions. Feel free to discuss with friends. Don't worry if you cannot answer a question fully as you will discuss the solutions in the class.

In problem set P0 we saw a convenient notation for complex vectors, $|v\rangle$. This problem set develops some useful properties of complex vectors.

5.0 Videos

Please watch this week's videos: V5.1, V5.2, V5.3a, V5.3b, V5.3c, V5.4

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

5.1 Hermitian conjugate

5.1.1

Define a complex N-dimensional vector

$$|v\rangle = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_N \end{pmatrix}. \tag{84}$$

Write expressions for

(a) the complex conjugate $(|v\rangle)^*$

ANS:

$$(|v\rangle)^* = \begin{pmatrix} v_1^* \\ v_2^* \\ v_3^* \\ \vdots \\ v_N^* \end{pmatrix}$$

dimensions $N \times 1$.

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

ANS:

$$(|v\rangle)^T = \begin{pmatrix} v_1, & v_2, & v_3, & \dots & v_N \end{pmatrix}$$

dimensions $1 \times N$.

What are the matrix dimensions of each object?

5.1.2

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

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

$$(|v\rangle)^\dagger \triangleq (|v\rangle)^{T*}\,. \tag{85}$$

By convention we write this

$$(|v\rangle)^\dagger \triangleq \langle v|. \tag{86}$$

ANS:

$$\left((|v\rangle)^T\right)^* = \left((|v\rangle)^*\right)^T = \left(\begin{pmatrix} v_1^*, & v_2^*, & v_3^*, & \ldots & v_N^* \end{pmatrix}\right).$$

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.

ANS:

$$\langle u|v\rangle = \begin{pmatrix} u_1^*, & u_2^*, & u_3^*, & \ldots & u_N^* \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_N \end{pmatrix} = u_1^* v_1 + u_2^* v_2 + u_3^* v_3 + \ldots + u_N^* v_N.$$

5.2.2

Show that

$$(\langle u|v\rangle)^* = \langle v|u\rangle. \tag{87}$$

ANS:

$$(\langle u|v\rangle)^* = \langle v|u\rangle = v_1^* u_1 + v_2^* u_2 + v_3^* u_3 + \ldots + v_N^* u_N$$

5.2.3

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

$$\||v\rangle\| = \sqrt{\langle v|v\rangle}. \tag{88}$$

ANS:

$$\begin{aligned}\||v\rangle\| &\triangleq \sqrt{|v_1|^2 + |v_2|^2 + \ldots + |v_N|^2} \\ &= \sqrt{\langle v|v\rangle}.\end{aligned}$$

5.2.4

Let

$$|v\rangle = \alpha|u\rangle + \beta|w\rangle \tag{89}$$

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.

ANS:

We require

$$\begin{aligned}1 &= \langle v|v\rangle \\ &= \left(\alpha^*\langle u| + \beta^*\langle w|\right)\left(\alpha|u\rangle + \beta|w\rangle\right) \\ &= |\alpha|^2 \cancelto{1}{\langle u|u\rangle} + |\beta|^2 \cancelto{1}{\langle w|w\rangle} + \alpha^*\beta \cancelto{0}{\langle u|w\rangle} + \alpha\beta^* \cancelto{0}{\langle w|u\rangle} \\ &= |\alpha|^2 + |\beta|^2 .\end{aligned}$$

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 $A|v\rangle$

ANS:

$N \times 1$

5.3.2 $\langle v|A$

ANS:

$1 \times N$

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

ANS:

1×1

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.

ANS:

$(N \times 1) \cdot (1 \times N) = N \times N$.

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

ANS:

$$|v\rangle\langle u| = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_N \end{pmatrix} \begin{pmatrix} u_1^*, & u_2^*, & u_3^*, & \dots & u_N^* \end{pmatrix}$$
$$= \begin{pmatrix} v_1 u_1^* & v_1 u_2^* & v_1 u_3^* & \dots & v_1 u_N^* \\ v_2 u_1^* & & & & \\ v_3 u_1^* & & & & \\ \vdots & & & \ddots & \\ v_N u_1^* & & & & v_N u_N^* \end{pmatrix}$$

as required.

5.5 Resolution of the identity

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

(a) What is $\langle e_i|e_j\rangle$?

ANS:

$$\langle e_i|e_j\rangle = \delta_{ij}$$

as the Kronecker delta δ_{ij} is 0 if $i \neq j$ (orthogonality) and 1 if $i = j$ (normality).

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

$$|v\rangle = \sum_{i=1}^{N} v_i |e_i\rangle \tag{90}$$

where

$$v_i = \langle e_i|v\rangle. \tag{91}$$

ANS: In perhaps more familiar notation, this simply reads

$$\boldsymbol{v} = \sum_{i=1}^{N} v_i \boldsymbol{e}_i$$

where

$$v_i = \boldsymbol{e}_i \cdot \boldsymbol{v}.$$

This is hopefully familiar: any vector can be written as a linear combination of basis vectors, provided the vectors span the space. If this is not familiar, give it a go in 2D with the basis

$$|e_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \ |e_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

(c) Two matrices A and B are equivalent iff

$$\langle u|A|v\rangle = \langle u|B|v\rangle \tag{92}$$

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

$$\mathbb{I} = \sum_{i=1}^{N} |e_i\rangle\langle e_i| \tag{93}$$

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

ANS:

$$|v\rangle = \sum_i |e_i\rangle\langle e_i|v\rangle$$

$$\downarrow$$

$$\langle u|\mathbb{I}|v\rangle = \langle u| \left(\sum_i |e_i\rangle\langle e_i| \right) |v\rangle.$$

5.6 Hermitian matrices

A Hermitian matrix is one which is equal to its Hermitian conjugate:

$$A^\dagger = A \tag{94}$$

i.e.

$$A^{T*} = A \tag{95}$$

or

$$A^*_{ij} = A_{ji}. \tag{96}$$

(a) Explain why this requires A to be square. We will assume this from now on.

ANS:

say A is $M \times N$. Then $A^\dagger$ must be $N \times M$, and if $A = A^\dagger$ we require $M = N$. QED.

(b) Recalling that

$$(AB)^T = B^T A^T \tag{97}$$

explain why

$$(A|v\rangle)^\dagger = \langle v|A^\dagger. \tag{98}$$

ANS:

$$(AB)^\dagger = B^\dagger A^\dagger.$$

Just think of $|v\rangle$ as an $N \times 1$ matrix, and let $B = |v\rangle$.

(c) The eigenvectors $|v_n\rangle$ and eigenvalues λ_n of matrix A are defined by the equation:

$$A|v_n\rangle = \lambda_n |v_n\rangle. \tag{99}$$

Show that

$$\langle v_n|A^\dagger = \lambda_n^* \langle v_n|. \tag{100}$$

ANS:

this follows from (b), noting that λ is a potentially complex scalar and that $\lambda^\dagger = \lambda^*$ since the transpose of a scalar is a scalar.

(d) By considering the object

$$\langle v_n| \left(A - A^\dagger\right) |v_n\rangle \tag{101}$$

prove that Hermitian matrices have real eigenvalues.

ANS:

$$\begin{aligned}
\langle v_n| \left(A - A^\dagger\right) |v_n\rangle &= \langle v_n|A|v_n\rangle - \langle v_n|A^\dagger|v_n\rangle \\
&= \langle v_n| \left(A|v_n\rangle\right) - \left(\langle v_n|A^\dagger\right) |v_n\rangle \\
&= \langle v_n| \left(\lambda_n|v_n\rangle\right) - \left(\langle v_n|\lambda_n^*\right) |v_n\rangle \\
&= \lambda_n \langle v_n|v_n\rangle - \lambda_n^* \langle v_n|v_n\rangle \\
&= \left(\lambda_n - \lambda_n^*\right) \langle v_n|v_n\rangle.
\end{aligned}$$

Since $A = A^\dagger$ for a Hermitian matrix, the left hand side must be zero. Therefore the right hand side is also zero. Since $\langle v_n|v_n\rangle$ is the length of the vector $|v_n\rangle$ which is only zero if the vector is the zero vector (which it's not), it must be the case that $\lambda_n = \lambda_n^*$ and λ_n is therefore real.

(e) Considering instead the object

$$\langle v_m| \left(A - A^\dagger\right) |v_n\rangle \tag{102}$$

prove the the eigenvectors of a Hermitian matrix are orthogonal to one another, provided no two eigenvalues are the same (the matrix is non-degenerate).

ANS:

$$\begin{aligned}
\langle v_m| \left(A - A^\dagger\right) |v_n\rangle &= \langle v_m|A|v_n\rangle - \langle v_m|A^\dagger|v_n\rangle \\
&= \langle v_m| \left(A|v_n\rangle\right) - \left(\langle v_m|A^\dagger\right) |v_n\rangle \\
&= \langle v_m| \left(\lambda_n|v_n\rangle\right) - \left(\langle v_m|\lambda_m^*\right) |v_n\rangle \\
&= \lambda_n\langle v_m|v_n\rangle - \lambda_m^*\langle v_m|v_n\rangle \\
&= \left(\lambda_n - \lambda_m^*\right) \langle v_m|v_n\rangle.
\end{aligned}$$

But we already showed that λ_n is real, so

$$\langle v_m| \left(A - A^\dagger\right) |v_n\rangle = \left(\lambda_n - \lambda_m\right) \langle v_m|v_n\rangle.$$

The left hand side is again zero. If no two eigenvalues are the same, $\lambda_n \neq \lambda_m$, and so we must have that $\langle v_m|v_n\rangle = 0$ for $n \neq m$.

(f) Assuming the eigenvalues of an $N \times N$ Hermitian matrix are non-degenerate, explain why the normalised eigenvectors must form a basis for the N-dimensional linear vector space.

ANS:

we just showed that the eigenvectors of such a matrix must be orthogonal to one another. If you have an N-dimensional space and N orthogonal vectors, they must span the space!

5.7 Matrices and eigenvalues

5.7.1

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

$$M = \sum_{i=1}^{N} \lambda_i|i\rangle\langle i| \tag{103}$$

where

$$M|i\rangle = \lambda_i|i\rangle. \tag{104}$$

ANS:

The eigenvectors of an N-dimensional Hermitian matrix form a complete orthonormal basis, so

$$\mathbb{I} = \sum_{i=1}^{N} |i\rangle\langle i|.$$

Acting with M from the left gives

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

5.7.2

Show this explicitly for each of the three Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{105}$$

ANS:

Eigenvectors; eigenvalues:

$$\begin{aligned}
\sigma_x &: \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}; \ 1, \ -1 \\
\sigma_y &: \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}; \ 1, \ -1 \\
\sigma_z &: \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}; \ 1, \ -1
\end{aligned}$$

therefore

$$\begin{aligned}
\sigma_x &= \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\begin{pmatrix} 1, & 1 \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix}\begin{pmatrix} 1, & -1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
\sigma_y &= \frac{1}{2}\begin{pmatrix} 1 \\ i \end{pmatrix}\begin{pmatrix} 1, - & i \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 1 \\ -i \end{pmatrix}\begin{pmatrix} 1, & i \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\
\sigma_z &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1, & 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0, & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\end{aligned}$$

5.8 Functions of matrices

A function of a matrix can be defined in terms of its Taylor series.

5.8.1

By comparing their Taylor series, show that

$$\exp(iAx) = \cos(Ax) + i\sin(Ax)\,. \tag{106}$$

5.8.2

Using the result that

$$\sigma_x^2 = \mathbb{I} \tag{107}$$

where σ_x is a Pauli matrix and $\mathbb{I}$ is the 2×2 identity matrix, show that

$$\exp(i\sigma_x x) = \cos(x)\,\mathbb{I} + i\sin(x)\,\sigma_x. \tag{108}$$

5.8.3

What are the eigenvectors of $\exp(i\sigma_x x)$? What are the corresponding eigenvalues?

5.8.4

Show that for

$$M = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \tag{109}$$

we have

$$\exp(M) = \mathbb{I} + M + \sum_{n=2}^{\infty} \frac{1}{n!} \begin{pmatrix} F_{n+1} & F_n \\ F_n & F_{n-1} \end{pmatrix} \tag{110}$$

where F_n is the n^{th} Fibonacci number.

5.9 Spin-1/2

5.9.1

The spin operators are defined to be

$$\hat{S}_i = \frac{\hbar}{2}\sigma_i \tag{111}$$

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

ANS:

Use the results of 5.7.2; the eigenvalues are multiplied by $\hbar/2$, and the eigenvectors are unchanged.

5.9.2

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 $|\downarrow_i\rangle$:

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

Using the result of equation 103 explain why each spin operator can be written in the form

$$\hat{S}_i = \frac{\hbar}{2}\left(|\uparrow_i\rangle\langle\uparrow_i| - |\downarrow_i\rangle\langle\downarrow_i|\right). \tag{112}$$

ANS:

just substitute in these eigenvalues and eigenvectors.

5.9.3

Show that we can write all operators in the spin-z basis as follows:

$$\hat{S}_x = \frac{\hbar}{2}\left(|\uparrow_z\rangle\langle\downarrow_z| + |\downarrow_z\rangle\langle\uparrow_z|\right) \tag{113}$$
$$\hat{S}_y = \frac{\hbar}{2}\left(i|\downarrow_z\rangle\langle\uparrow_z| - i|\uparrow_z\rangle\langle\downarrow_z|\right) \tag{114}$$
$$\hat{S}_z = \frac{\hbar}{2}\left(|\uparrow_z\rangle\langle\uparrow_z| - |\downarrow_z\rangle\langle\downarrow_z|\right). \tag{115}$$

If you see spins written without the direction designated it is conventional to define them along z in this way.

ANS:

All spins are now along z: $|\uparrow_i\rangle = |\uparrow_z\rangle$. The $\hat{S}_z$ equation is unchanged. Each spin vector can be written as a linear combination of the two spin-z vectors:

$$
\begin{aligned}
|\uparrow_x\rangle &= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}\\
&= \frac{1}{\sqrt{2}}\left(\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\right)\\
&= \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle + |\downarrow_z\rangle\right)
\end{aligned}
$$

and so on. Therefore

$$
|\uparrow_x\rangle\langle\uparrow_x| = \frac{1}{2}\left(|\uparrow_z\rangle + |\downarrow_z\rangle\right)\left(\langle\uparrow_z| + \langle\downarrow_z|\right)
$$

and doing the same for the various terms in $\hat{S}_x$ and $\hat{S}_y$ gives the result.

5.9.4

Use the forms just derived to show that

$$
\left[\hat{S}_i, \hat{S}_j\right] = i\hbar\sum_{k=1}^{3}\epsilon_{ijk}\hat{S}_k \tag{116}
$$

where the directions x, y, z are numbered 1, 2, and 3 respectively, and ϵ_{ijk} is the Levi-Civita symbol defined by

$$
\epsilon_{ijk} = \begin{cases} 0, \text{ any of } i,j,k \text{ equal} \\ 1,\ ijk = 123 \text{ or cyclic permutations} \\ -1,\ ijk = 321 \text{ or cyclic permutations.} \end{cases} \tag{117}
$$

ANS:

Three terms need to be checked. One is

$$
\left[\hat{S}_x, \hat{S}_y\right]
$$

and the other two follow by cyclic permutation of indices. For this case we have

$$
\begin{aligned}
\left[\hat{S}_x, \hat{S}_y\right] &= \hat{S}_x\hat{S}_y - \hat{S}_y\hat{S}_x \\
&= \frac{\hbar}{2}\left(|\uparrow_z\rangle\langle\downarrow_z| + |\downarrow_z\rangle\langle\uparrow_z|\right)\frac{\hbar}{2}\left(i|\downarrow_z\rangle\langle\uparrow_z| - i|\uparrow_z\rangle\langle\downarrow_z|\right) \\
&- \frac{\hbar}{2}\left(i|\downarrow_z\rangle\langle\uparrow_z| - i|\uparrow_z\rangle\langle\downarrow_z|\right)\frac{\hbar}{2}\left(|\uparrow_z\rangle\langle\downarrow_z| + |\downarrow_z\rangle\langle\uparrow_z|\right) \\
&= \frac{\hbar^2}{4}\left(i|\uparrow_z\rangle\langle\downarrow_z|\downarrow_z\rangle\langle\uparrow_z| - i|\uparrow_z\rangle\langle\downarrow_z|\uparrow_z\rangle\langle\downarrow_z| + i|\downarrow_z\rangle\langle\uparrow_z|\downarrow_z\rangle\langle\uparrow_z| - i|\downarrow_z\rangle\langle\uparrow_z|\uparrow_z\rangle\langle\downarrow_z|\right)
\end{aligned}
$$

where the last line is found by multiplying out, and

$$
\begin{aligned}
\left[\hat{S}_x, \hat{S}_y\right] &= \frac{i\hbar^2}{4}\left(|\uparrow_z\rangle\cancelto{1}{\langle\downarrow_z|\downarrow_z\rangle}\langle\uparrow_z| - |\uparrow_z\rangle\cancelto{0}{\langle\downarrow_z|\uparrow_z\rangle}\langle\downarrow_z| + |\downarrow_z\rangle\cancelto{0}{\langle\uparrow_z|\downarrow_z\rangle}\langle\uparrow_z| - |\downarrow_z\rangle\cancelto{1}{\langle\uparrow_z|\uparrow_z\rangle}\langle\downarrow_z|\right) \\
&= \frac{i\hbar^2}{4}\left(|\uparrow_z\rangle\langle\uparrow_z| - |\downarrow_z\rangle\langle\downarrow_z|\right) \\
&= \frac{i\hbar}{2}\hat{S}_z
\end{aligned}
$$

which is the desired result.

6 Operators and observables

Bring solutions along to the class at 10am on 9/11/20.

Questions marked # are beyond the syllabus. We may discuss them in the class if there is time.

Attempt all questions. Feel free to discuss with friends. Don't worry if you cannot answer a question fully as you will discuss the solutions in the class.

6.0 Videos

Please watch this week's videos: V6.1, V6.2, V6.3, V6.4.

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

6.1 The Heisenberg picture

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

$$\hat{A}_H(t) = \exp\left(i\hat{H}t/\hbar\right)\hat{A}_S \exp\left(-i\hat{H}t/\hbar\right). \quad (118)$$

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:

$$|\psi_S(t)\rangle = \exp\left(-i\hat{H}t/\hbar\right)|\psi_S(0)\rangle = \exp\left(-i\hat{H}t/\hbar\right)|\psi_H\rangle \quad (119)$$

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

$$\langle\varphi|\hat{A}|\psi\rangle = \langle\varphi|\hat{B}|\psi\rangle \quad \forall|\varphi\rangle, |\psi\rangle. \quad (120)$$

Show that

$$\langle\varphi_H|\hat{A}_H(t)|\psi_H\rangle = \langle\varphi_S(t)|\hat{A}_S|\psi_S(t)\rangle \quad (121)$$

and hence the two pictures are equivalent.

ANS:

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

6.1.2

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

$$\left[i\hbar\partial_t, \hat{H}\right] = 0. \tag{122}$$

ANS:

they are the same operator.

(b) Why must

$$\left[\hat{H}, f\left(\hat{H}\right)\right] = 0 \tag{123}$$

for any function f?

ANS:

$f\left(\hat{H}\right)$ can be written as a Taylor series in which each term is a power of $\hat{H}$. Since $\left[\hat{H}, \hat{H}^n\right] = 0$ for integer n the result follows.

6.1.3

Hence derive the Heisenberg equation of motion:

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

ANS:

$$\begin{aligned}
i\hbar\frac{\partial\hat{A}_H(t)}{\partial t} &= \left(i\hbar\frac{\partial}{\partial t}\exp\left(-i\hat{H}t/\hbar\right)\right)\hat{A}_S\exp\left(i\hat{H}t/\hbar\right) + \exp\left(-i\hat{H}t/\hbar\right)\hat{A}_S\left(i\hbar\frac{\partial}{\partial t}\exp\left(i\hat{H}t/\hbar\right)\right) \\
\frac{\partial\hat{A}_H(t)}{\partial t} &= -\frac{i}{\hbar}\hat{H}\exp\left(-i\hat{H}t/\hbar\right)\hat{A}_S\exp\left(i\hat{H}t/\hbar\right) + \exp\left(-i\hat{H}t/\hbar\right)\hat{A}_S\left(\frac{i}{\hbar}\hat{H}\exp\left(i\hat{H}t/\hbar\right)\right) \\
&= -\frac{i}{\hbar}\hat{H}\hat{A}_H(t) + \frac{i}{\hbar}\hat{A}_H(t)\hat{H} \\
i\hbar\frac{\partial\hat{A}_H(t)}{\partial t} &= \left[\hat{A}_H(t), \hat{H}\right] \\
i\hbar\frac{\mathrm{d}\hat{A}_H(t)}{\mathrm{d}t} &= \left[\hat{A}_H(t), \hat{H}\right].
\end{aligned}$$

6.1.4

Use this result to prove Ehrenfest's theorem:

$$i\hbar\frac{\mathrm{d}\langle\hat{A}\rangle}{\mathrm{d}t}=\langle\left[\hat{A},\hat{H}\right]\rangle. \tag{125}$$

ANS:

$$\begin{aligned}
i\hbar\frac{\mathrm{d}\hat{A}_H\left(t\right)}{\mathrm{d}t} &= \left[\hat{A}_H\left(t\right),\hat{H}\right]\\
i\hbar\langle\psi_H|\frac{\mathrm{d}\hat{A}_H\left(t\right)}{\mathrm{d}t}|\psi_H\rangle &= \langle\psi_H|\left[\hat{A}_H\left(t\right),\hat{H}\right]|\psi_H\rangle\\
&\downarrow |\psi_H\rangle \text{ time independent}\\
i\hbar\frac{\mathrm{d}\langle\psi_H|\hat{A}_H\left(t\right)|\psi_H\rangle}{\mathrm{d}t} &= \langle\psi_H|\left[\hat{A}_H\left(t\right),\hat{H}\right]|\psi_H\rangle\\
i\hbar\frac{\mathrm{d}\langle\hat{A}\left(t\right)\rangle}{\mathrm{d}t} &= \langle\left[\hat{A}_H\left(t\right),\hat{H}\right]\rangle.
\end{aligned}$$

6.1.5

Prove Ehrenfest's theorem another way, by taking the partial time derivative of the expectation value of a time-independent operator in the Schrödinger picture:

$$\langle\varphi_S\left(t\right)|\hat{A}_S|\psi_S\left(t\right)\rangle. \tag{126}$$

ANS:

the general solution including time-dependent $\hat{A}$ is

$$\begin{aligned}
\left(\frac{\partial}{\partial t}\right)\langle\psi\left(t\right)|\hat{A}\left(t\right)|\psi\left(t\right)\rangle &= \left(\frac{\partial}{\partial t}\langle\psi\left(t\right)|\right)\hat{A}\left(t\right)|\psi\left(t\right)\rangle+\langle\psi\left(t\right)|\left(\frac{\partial}{\partial t}\hat{A}\left(t\right)\right)|\psi\left(t\right)\rangle+\langle\psi\left(t\right)|\hat{A}\left(t\right)\left(\frac{\partial}{\partial t}|\psi\left(t\right)\rangle\right)\\
\frac{\partial\langle\hat{A}\left(t\right)\rangle}{\partial t} &= \left(\frac{i}{\hbar}\langle\psi\left(t\right)|\hat{H}\right)\hat{A}\left(t\right)|\psi\left(t\right)\rangle+\langle\frac{\partial\hat{A}\left(t\right)}{\partial t}\rangle+\langle\psi\left(t\right)|\hat{A}\left(t\right)\left(\frac{-i}{\hbar}\hat{H}|\psi\left(t\right)\rangle\right)\\
&\downarrow \text{lhs only depends on } t\\
i\hbar\frac{\mathrm{d}\langle\hat{A}\left(t\right)\rangle}{\mathrm{d}t} &= -\langle\psi\left(t\right)|\hat{H}\hat{A}\left(t\right)|\psi\left(t\right)\rangle+\langle\frac{\partial\hat{A}\left(t\right)}{\partial t}\rangle+\langle\psi\left(t\right)|\hat{A}\left(t\right)\hat{H}|\psi\left(t\right)\rangle\\
&= \langle\hat{A}\left(t\right)\hat{H}-\hat{H}\hat{A}\left(t\right)\rangle+\langle\frac{\partial\hat{A}\left(t\right)}{\partial t}\rangle\\
&= \langle\left[\hat{A}\left(t\right),\hat{H}\right]\rangle+\langle\frac{\partial\hat{A}\left(t\right)}{\partial t}\rangle.
\end{aligned}$$

If $\hat{A}$ is time independent the last term disappears.

6.1.6

In fact operators in the Schrödinger picture can have their own time dependences; for example, we might be interested in a potential which varies with time. Such cases are beyond the syllabus for this course. Show that if $\hat{A}_S(t)$ has a time dependence the Heisenberg equation of motion reads

$$i\hbar\frac{\mathrm{d}\hat{A}_H(t)}{\mathrm{d}t} = \left[\hat{A}_H(t), \hat{H}\right] + i\hbar \exp\left(-i\hat{H}t/\hbar\right)\left(\frac{\partial\hat{A}_S(t)}{\partial t}\right)\exp\left(i\hat{H}t/\hbar\right). \tag{127}$$

ANS:

see previous answer in the general case.

6.2 The Heisenberg Uncertainty Principle

6.2.1

State the (generalised) Heisenberg uncertainty principle, explaining the various terms in the expression.

ANS:

$$\sigma_{\hat{A}}\sigma_{\hat{B}} \geq \frac{1}{2}\left|\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right|$$

where

$$\sigma_{\hat{A}} \triangleq \sqrt{\left\langle\hat{A}^2\right\rangle - \left\langle\hat{A}\right\rangle^2}$$

is the ‘uncertainty’ (standard deviation).

6.2.2

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

$$[\hat{x},\hat{p}] = i\hbar\hat{\mathbb{I}} \tag{128}$$

where $\hat{\mathbb{I}}$ 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.

ANS:

$$\begin{aligned}\sigma_{\hat{x}}\sigma_{\hat{p}} &\geq \frac{1}{2}\left|\langle[\hat{x},\hat{p}]\rangle\right| \\ &\geq \frac{1}{2}\left|i\hbar\right| \\ &\geq \frac{\hbar}{2}.\end{aligned}$$

6.2.3

Using the commutation relation between spin operators:

$$\left[\hat{S}_x, \hat{S}_y\right] = i\hbar\hat{S}_z \tag{129}$$

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

ANS:

$$\begin{aligned}\sigma_{\hat{S}_x}\sigma_{\hat{S}_y} &\geq \frac{1}{2}\left|\left\langle\left[\hat{S}_x, \hat{S}_y\right]\right\rangle\right| \\ &\geq \frac{1}{2}\left|\left\langle i\hbar\hat{S}_z\right\rangle\right| \\ &\geq \frac{\hbar}{2}\left|\left\langle\hat{S}_z\right\rangle\right|.\end{aligned}$$

6.2.4

Give a physical explanation for the mathematical results you just derived.

ANS:

the precise answer depends on your interpretation of quantum mechanics. It is agreed that the expression sets a precise lower bound on the simultaneous experimental information we can have about any two observables whose operators do not commute. Whether this is because the information does not exist, or whether it's because we just can't know it ourselves, or whether something happens between the quantum scale and the macroscopic scale, is then an interpretational issue.

6.3 The correspondence principle

The correspondence principle is the idea that classical mechanics should be returned as the $\hbar \to 0$ limit of quantum mechanics ($\hbar$ is constant, but if it could vary, setting it to zero would result in a classical universe). Part of this is the idea that quantum results should approximate classical results at large quantum numbers. Ehrenfest's theorem is often used as evidence in support of this idea.

6.3.1

Prove the general matrix result

$$[AB, C] = A[B, C] + [A, C]B. \tag{130}$$

ANS:

Either expand both sides, or use:

$$\begin{aligned}[AB, C] &= ABC - CAB \\ &= ABC - CAB - ACB + ACB \\ &= ABC - ACB + ACB - CAB \\ &= A(BC - CB) + (AC - CA)B \\ &= A[B, C] + [A, C]B.\end{aligned}$$

6.3.2

Using the canonical commutation relation show that

$$\left[\hat{x}^2, \hat{p}\right] = 2i\hbar\hat{x}. \tag{131}$$

ANS:

using the above result,

$$\begin{aligned}\left[\hat{x}^2, \hat{p}\right] &= \hat{x}[\hat{x}, \hat{p}] + [\hat{x}, \hat{p}]\hat{x} \\ &= i\hbar\hat{x}\hat{\mathbb{I}} + i\hbar\hat{\mathbb{I}}\hat{x} \\ &= 2i\hbar\hat{x}.\end{aligned}$$

6.3.3

Another way to show the same result is by 'pulling through' the $\hat{p}$ operator, which is a very useful trick. Noting that

$$\hat{p}\hat{x} = \hat{x}\hat{p} - [\hat{x}, \hat{p}] \tag{132}$$

by the definition of the commutator, you can pull the $\hat{p}$ operator through the $\hat{x}$ operator, switching their order, at the cost of subtracting the commutator.

a) Show that

$$\hat{p}\hat{x}^2 = (\hat{x}\hat{p} - [\hat{x}, \hat{p}])\,\hat{x} \tag{133}$$

and therefore

$$\hat{p}\hat{x}^2 = \hat{x}\hat{p}\hat{x} - i\hbar\hat{x}. \tag{134}$$

b) Repeating the same technique, show that

$$\hat{p}\hat{x}^2 = \hat{x}^2\hat{p} - 2i\hbar\hat{x}. \tag{135}$$

c) Therefore deduce that

$$\left[\hat{x}^2, \hat{p}\right] = 2i\hbar\hat{x}. \tag{136}$$

6.3.4

This technique of pulling through the operator can be used to prove a more general result.

a) Show that

$$\hat{p}\hat{x}^n = \hat{x}\hat{p}\hat{x}^{n-1} - i\hbar\hat{x}^{n-1} \tag{137}$$

ANS:

$$\begin{aligned}\hat{p}\hat{x}^n &= (\hat{x}\hat{p} - [\hat{x}, \hat{p}])\,\hat{x}^{n-1} \\ &= (\hat{x}\hat{p} - i\hbar)\,\hat{x}^{n-1} \\ &= \hat{x}\hat{p}\hat{x}^{n-1} - i\hbar\hat{x}^{n-1}.\end{aligned}$$

b) Noting that the first term on the right-hand side contains $\hat{p}\hat{x}^{n-1}$, and that you have already worked this out in (a) (replacing n with $n-1$), show that

$$\hat{p}\hat{x}^n = \hat{x}^2\hat{p}\hat{x}^{n-2} - 2i\hbar\hat{x}^{n-1}. \tag{138}$$

ANS:

$$\begin{aligned}\hat{p}\hat{x}^{n} &= \hat{x}\left(\hat{p}\hat{x}^{n-1}\right) - i\hbar\hat{x}^{n-1} \\ &= \hat{x}\left(\hat{x}\hat{p}\hat{x}^{n-2} - i\hbar\hat{x}^{n-2}\right) - i\hbar\hat{x}^{n-1} \\ &= \hat{x}^{2}\hat{p}\hat{x}^{n-2} - i\hbar\hat{x}^{n-1} - i\hbar\hat{x}^{n-1} \\ &= \hat{x}^{2}\hat{p}\hat{x}^{n-2} - 2i\hbar\hat{x}^{n-1}.\end{aligned}$$

c) Therefore explain why

$$\hat{p}\hat{x}^{n} = \hat{x}^{n}\hat{p} - ni\hbar\hat{x}^{n-1} \tag{139}$$

and deduce that

$$[\hat{x}^{n}, \hat{p}] = ni\hbar\hat{x}^{n-1}. \tag{140}$$

ANS:

The stated identity just follows from repeating the process n times.

$$\begin{aligned}[\hat{x}^{n}, \hat{p}] &= \hat{x}^{n}\hat{p} - \hat{p}\hat{x}^{n} \\ &= \hat{x}^{n}\hat{p} - \left(\hat{x}^{n}\hat{p} - ni\hbar\hat{x}^{n-1}\right) \\ &= ni\hbar\hat{x}^{n-1}.\end{aligned}$$

d) # How might you denote the result of

$$\frac{1}{i\hbar}\left[f\left(\hat{x}\right), \hat{p}\right]? \tag{141}$$

ANS:

since $f\left(\hat{x}\right)$ can be defined by its Taylor series:

$$f\left(\hat{x}\right) = a_0\hat{\mathbb{I}} + \sum_{n=1}^{\infty}\frac{a_n}{n!}\hat{x}^{n}$$

we have

$$\frac{1}{i\hbar}\left[f\left(\hat{x}\right),\hat{p}\right] = \sum_{n=1}^{\infty}\frac{a_n}{(n-1)!}\hat{x}^{(n-1)}$$
$$= f'\left(\hat{x}\right).$$

6.3.5

Using Ehrenfest's theorem, show that

$$\frac{\mathrm{d}\left\langle\hat{x}\right\rangle}{\mathrm{d}t} = \frac{\left\langle\hat{p}\right\rangle}{m}. \tag{142}$$

This suggests that the expectation values of quantum operators obey the classical equation $\dot{x} = p/m$, even if quantum operators do not.

ANS:

$$\begin{aligned}\frac{\mathrm{d}\langle\hat{x}\rangle}{\mathrm{d}t} &= \frac{-i}{\hbar}\langle\left[\hat{x},\hat{H}\right]\rangle\\ &= \frac{-i}{\hbar}\langle\left[\hat{x},\frac{1}{2m}\hat{p}^2+V\left(\hat{x}\right)\right]\rangle\\ &= \frac{-i}{2m\hbar}\langle\left[\hat{x},\hat{p}^2\right]\rangle\\ &= \frac{-i}{2m\hbar}\langle\left[\hat{x},\hat{p}\right]\hat{p}+\hat{p}\left[\hat{x},\hat{p}\right]\rangle\\ &= \frac{-i}{2m\hbar}\langle 2i\hbar\hat{p}\rangle\\ &= \left\langle\hat{p}\right\rangle/m.\end{aligned}$$

6.3.6

a) Using Ehrenfest's theorem, and defining $V\left(\hat{x}\right)$ by its Taylor series, show that

$$\frac{\mathrm{d}\left\langle\hat{p}\right\rangle}{\mathrm{d}t} = -\left\langle V'\left(\hat{x}\right)\right\rangle \tag{143}$$

where $f'\left(x\right) = \partial f\left(x\right)/\partial x$.

b) Which classical equation of motion does this resemble?

c) Combined with the previous result it is tempting to say that the expectation values of quantum operators obey classical equations of motion. What feature of this second equation makes such a statement inaccurate?

d) Find a condition on the expectation values of the power of the position operator for which the statement is accurate.

e) Show that this condition is obeyed in the case of a quadratic potential.

ANS:

a)

$$\begin{aligned}\frac{\mathrm{d}\langle\hat{p}\rangle}{\mathrm{d}t} &= -\frac{i}{\hbar}\left\langle\left[\hat{p},\hat{H}\right]\right\rangle \\ &= -\frac{i}{\hbar}\left\langle\left[\hat{p},\frac{1}{2m}\hat{p}^2+V(\hat{x})\right]\right\rangle \\ &= -\frac{i}{\hbar}\left\langle\left[\hat{p},V(\hat{x})\right]\right\rangle\end{aligned}$$

Now use the fact that a function of an operator is defined by its Taylor series:

$$V(\hat{x}) \triangleq a_0\hat{\mathbb{I}} + \sum_{n=1}^{\infty}\frac{a_n}{n!}\hat{x}^n$$

and the result from above, that

$$[\hat{p},\hat{x}^n] = -i\hbar n\hat{x}^{n-1}$$

to deduce

$$\begin{aligned}[\hat{p},V(\hat{x})] &= a_0\overbrace{\left[\hat{p},\hat{\mathbb{I}}\right]}^{0} + \sum_{n=1}^{\infty}\frac{a_n}{n!}[\hat{p},\hat{x}^n] \\ &= -i\hbar\sum_{n=1}^{\infty}\frac{a_n}{(n-1)!}\hat{x}^{n-1} \\ &= -i\hbar V'(\hat{x})\end{aligned}$$

where the prime indicates the derivative of the function. Therefore

$$\begin{aligned}\frac{\mathrm{d}\langle\hat{p}\rangle}{\mathrm{d}t} &= -\frac{i}{\hbar}\left\langle\left[\hat{p},\hat{H}\right]\right\rangle \\ &= -\left\langle V'(\hat{x})\right\rangle\end{aligned}$$

or in 3D

$$\frac{\mathrm{d}\langle\hat{p}\rangle}{\mathrm{d}t} = -\left\langle\nabla V(\hat{x})\right\rangle$$

where the ∇ is understood to act on the function V.

b) it resembles Newton's second law

c) For the statement to be accurate, the equation would need to be

$$\frac{\mathrm{d}\langle\hat{p}\rangle}{\mathrm{d}t} = -\nabla V\left(\langle\hat{x}\rangle\right).$$

d) For the statements to be equivalent, we require

$$\langle V'(\hat{x})\rangle = V'\left(\langle\hat{x}\rangle\right).$$

Defining V by its Taylor series again:

$$V(\hat{x}) = a_0\mathbb{I} + \sum_{n=1}^{\infty}\frac{a_n}{n!}\hat{x}^n$$

we have

$$V'(\hat{x}) = \sum_{n=1}^{\infty}\frac{a_n}{(n-1)!}\hat{x}^{n-1}$$

and so the required condition is that

$$\langle V'(\hat{x})\rangle = V'\left(\langle\hat{x}\rangle\right)$$
$$\sum_{n=1}^{\infty}\frac{a_n}{(n-1)!}\left\langle\hat{x}^{n-1}\right\rangle = \sum_{n=1}^{\infty}\frac{a_n}{(n-1)!}\langle\hat{x}\rangle^{n-1}$$

i.e.

$$\left\langle\hat{x}^{n-1}\right\rangle = \langle\hat{x}\rangle^{n-1} \quad \forall n \geq 1$$
$$\left\langle\hat{x}^{n}\right\rangle = \langle\hat{x}\rangle^{n} \quad \forall n \geq 2.$$

e) For a quadratic potential,

$$
\begin{aligned}
\frac{\mathrm{d}\langle\hat{p}\rangle}{\mathrm{d}t} &= -\frac{i}{\hbar}\left\langle\left[\hat{p}, \frac{\hat{p}^2}{2m} + \alpha\hat{x}^2 + \beta\hat{x}\right]\right\rangle \\
&= -\frac{i}{\hbar}\left\langle\left[\hat{p}, \alpha\hat{x}^2 + \beta\hat{x}\right]\right\rangle \\
&= -\frac{i}{\hbar}\left\langle\alpha\left[\hat{p}, \hat{x}^2\right] + \beta\left[\hat{p}, \hat{x}\right]\right\rangle \\
&= -\frac{i}{\hbar}\left\langle\alpha\left[\hat{p}, \hat{x}\right]\hat{x} + \alpha\hat{x}\left[\hat{p}, \hat{x}\right] + \beta\left[\hat{p}, \hat{x}\right]\right\rangle \\
&= \left\langle 2\alpha\hat{x} + \beta\mathbb{I}\right\rangle \\
&= 2\alpha\left\langle\hat{x}\right\rangle + \beta
\end{aligned}
$$

and if

$$V\left(\hat{x}\right) = \alpha\hat{x}^2 + \beta\hat{x}$$

then

$$V'\left(\hat{x}\right) = 2\alpha\hat{x} + \beta$$

so in this case

$$\left\langle V'\left(\hat{x}\right)\right\rangle = V'\left(\left\langle\hat{x}\right\rangle\right).$$

6.4 Joint eigenvectors

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

6.4.1

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

$$A|v_n\rangle = a_n|v_n\rangle \tag{144}$$

$$B|v_n\rangle = b_n|v_n\rangle. \tag{145}$$

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

$$[A, B] = 0. \tag{146}$$

ANS:

$$AB|v_n\rangle = Ab_n|v_n\rangle = a_nb_n|v_n\rangle$$
$$BA|v_n\rangle = Ba_n|v_n\rangle = a_nb_n|v_n\rangle$$

therefore

$$[A, B]\,|v_n\rangle = 0$$

and since neither A nor B is zero, and $|v_n\rangle$ cannot be zero, the result holds.

6.4.2

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

$$A|a_n\rangle = a_n|a_n\rangle. \tag{147}$$

Show that if

$$[A, B] = 0 \tag{148}$$

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

ANS:

$$A|a_n\rangle = a_n|a_n\rangle$$
$$\downarrow B \rightarrow$$
$$BA|a_n\rangle = a_nB|a_n\rangle$$
$$\downarrow [A, B] = 0$$
$$A\left(B|a_n\rangle\right) = a_n\left(B|a_n\rangle\right)$$

but this equation defines $B|a_n\rangle$ to be proportional to an eigenvalue of A with eigenvalue a_n *i.e.*

$$B|a_n\rangle \propto |a_n\rangle.$$

Inserting an arbitrary constant of proportionality this is just an eigenvalue equation for B:

$$B|a_n\rangle = b_n|a_n\rangle.$$

6.4.3

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

6.5 Quantum numbers

6.5.1

Explain what is meant by a quantum number.

ANS:

A physical observable which does not change in time (i.e. a conserved quantity). For an operator $\hat{A}$, the expectation value is time-independent:

$$\frac{\mathrm{d}\left\langle \hat{A} \right\rangle}{\mathrm{d}t} = 0.$$

6.5.2

Using Ehrenfest's theorem, explain why, for an observable to be a quantum number, the corresponding operator must commute with the Hamiltonian.

ANS:

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

therefore if $\frac{\mathrm{d}\langle \hat{A} \rangle}{\mathrm{d}t} = 0$

$$\left\langle \left[\hat{A}, \hat{H}\right] \right\rangle = 0$$

and so

$$\left[\hat{A}, \hat{H}\right] = 0$$

since $|\psi\rangle$ used to take the expectation value is never the zero vector.

6.5.3

Hence explain why energy is always a good quantum number.

ANS:

the energy operator is the Hamiltonian, and $\left[\hat{H}, \hat{H}\right] = 0$.

6.5.4

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

ANS:

We showed in the previous question that if two operators commute their eigenvalues can be known simultanously. Hence for $\mathrm{d}\left\langle \hat{A} \right\rangle/\mathrm{d}t = 0$ we have $\left[\hat{A}, \hat{H}\right] = 0$ and we can know the eigenvalues of $\hat{A}$ alongside the eigenvalues of $\hat{H}$, i.e. the energy.

6.6 # Energy-time uncertainty

The energy-time uncertainty relation cannot be made precise like other uncertainty relations, because there is no time operator in quantum mechanics. This question explores one approach to making a precise statement of the energy-time uncertainty due to Mandelstam and Tamm.

6.6.1

List some reasons we expect there to be some kind of uncertainty relation between energy and time.

ANS:

(e.g.)

- if the uncertainty in time of emission of a particle is smaller, the uncertainty in its energy is larger
- the 'width' of a particle resonance is inversely proportional to its lifetime
- energy and time are Fourier conjugate to one another

6.6.2

Use Ehrenfest's theorem and the generalised Heisenberg uncertainty equation to show that

$$\sigma_{\hat{H}} \left(\frac{\sigma_{\hat{A}}}{\left| \frac{\mathrm{d}\langle A \rangle}{\mathrm{d}t} \right|} \right) \geq \frac{\hbar}{2} \tag{149}$$

where $\sigma_{\hat{A}}$ is the uncertainty in $\hat{A}$, defined in the usual way as the standard deviation, $\hat{H}$ is the Hamiltonian, and $\hat{A}$ is an arbitrary operator.

ANS:

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

therefore

$$\sigma_{\hat{H}}\sigma_{\hat{A}} \geq \frac{1}{2}\left|\left\langle\left[\hat{H},\hat{A}\right]\right\rangle\right|$$
$$\geq \frac{\hbar}{2}\left|\frac{\mathrm{d}\langle\hat{A}\rangle}{\mathrm{d}t}\right|$$

and

$$\sigma_{\hat{H}}\frac{\sigma_{\hat{A}}}{\left|\frac{\mathrm{d}\langle A\rangle}{\mathrm{d}t}\right|} \geq \frac{\hbar}{2}.$$

6.6.3

Suggest an interpretation of the formula you have just found.

ANS:

there is an uncertainty between the energy (given by the standard deviation of $\hat{H}$ in the $|\psi\rangle$ basis, $\sigma_{\hat{H}}$) and a quantity which can be interpreted as the average time taken for operator $\hat{A}$ to change by one standard deviation, and therefore to change by a measurable amount.

7 Quantum mechanics

Bring solutions along to the class at 10am on 16/11/20.

Questions marked # are beyond the syllabus. We may discuss them in the class if there is time.

Attempt all questions. Feel free to discuss with friends. Don't worry if you cannot answer a question fully as you will discuss the solutions in the class.

7.0 Videos

Please watch this week's videos: V7.1, V7.2, V7.3, V7.4, V7.5.

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

7.1 Infinite-dimensional Hilbert spaces

7.1.1

State the axioms of linear vector spaces (recall PS0), and show that they are satisfied by complex functions $f(x)$. We are therefore justified in using vector notation to decribe functions: $|f\rangle$, or, in the position basis specifically, $\langle x|f\rangle = f(x)$.

ANS:

$\forall \{|x\rangle, |y\rangle, |z\rangle\} \in V;\ \alpha, \beta \in \mathbb{C}:$

1. $|x\rangle + |y\rangle \in V$
2. $(|x\rangle + |y\rangle) + |z\rangle = |x\rangle + (|y\rangle + |z\rangle)$
3. $\exists |0\rangle \in V:\ |x\rangle + |0\rangle = |0\rangle + |x\rangle = |x\rangle$
4. $\exists (-|x\rangle) \in V:\ |x\rangle + (-|x\rangle) = |0\rangle$
5. $|x\rangle + |y\rangle = |y\rangle + |x\rangle$
6. $\alpha|x\rangle \in V$
7. $\alpha(|x\rangle + |y\rangle) = \alpha|x\rangle + \alpha|y\rangle$
8. $(\alpha + \beta)|x\rangle = \alpha|x\rangle + \beta|x\rangle$
9. $\alpha(\beta|x\rangle) = (\alpha\beta)|x\rangle$
10. $1|x\rangle = |x\rangle$.

All trivially satisfied by $f(x)$.

7.1.2

State the axioms of an 'inner product space'. 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

$$\langle f|g\rangle \triangleq \int_{-\infty}^{\infty} f(x)^* g(x)\,\mathrm{d}x. \tag{150}$$

ANS:

1. $\langle a|b\rangle = (\langle b|a\rangle)^*$

2. $\langle a|a\rangle \geq 0$, equality iff $|a\rangle = |0\rangle$
3. $\langle c|\left(\alpha|a\rangle + \beta|b\rangle\right) = \alpha\langle c|a\rangle + \beta\langle c|b\rangle$.
1. $\left(\int b\left(x\right)^{*} a\left(x\right) \mathrm{d}x\right)^{*} = \int a\left(x\right)^{*} b\left(x\right) \mathrm{d}x$✓
2. $\int \left|a\left(x\right)\right|^{2} \mathrm{d}x$ obeys as $\left|a\left(x\right)\right|$ obeys.
3. $\int c\left(x\right)^{*}\left(\alpha a\left(x\right) + \beta b\left(x\right)\right) \mathrm{dx} = \alpha \int c\left(x\right)^{*} a\left(x\right) \mathrm{d}x + \beta \int c\left(x\right)^{*} b\left(x\right) \mathrm{d}x$.

7.1.3

Explain why the norm of any quantum state $|\psi\rangle$ must be one. State this restriction in terms of the wavefunction $\langle x|\psi\rangle = \psi\left(x\right)$. This last property, square-integrability, defines the space of wavefunctions to be an infinite-dimensional Hilbert space.

ANS:

$$\begin{aligned} 1 &= \langle\psi|\psi\rangle \\ &= \int \langle\psi|x\rangle\langle x|\psi\rangle \mathrm{d}x \\ &= \int \left|\psi\left(x\right)\right|^{2} \mathrm{d}x \end{aligned}$$

which is true as the particle must exist somewhere.

7.2 Fourier transforms

In general the Fourier transform (FT) and inverse transform (FT^{-1}) of a pair of functions in variables ξ and t

$$\tilde{f}\left(\xi\right) = \mathrm{FT}\left[f\left(t\right)\right] \tag{151}$$

$$f\left(t\right) = \mathrm{FT}^{-1}\left[\tilde{f}\left(\xi\right)\right] \tag{152}$$

are defined as:

$$\tilde{f}\left(\xi\right) = \int_{-\infty}^{\infty} f\left(t\right) \exp\left(-2\pi i\xi t\right) \mathrm{d}t \tag{153}$$

$$f\left(t\right) = \int_{-\infty}^{\infty} \tilde{f}\left(\xi\right) \exp\left(2\pi i\xi t\right) \mathrm{d}\xi \tag{154}$$

[t need not be time; ξ and t are just any pair of Fourier-conjugate variables]. In quantum mechanics it is convenient to rescale the variables to

$$2\pi\xi t \rightarrow px/\hbar \tag{155}$$

so that we are working with plane waves. One way to achieve this is to define

$$\xi \triangleq p/\sqrt{2\pi\hbar} \tag{156}$$
$$t \triangleq x/\sqrt{2\pi\hbar}. \tag{157}$$

There are other choices, akin to the usual ambiguity in the placement of the 2π factors in Fourier transforms.

7.2.1

For a suitable definition of $\phi(x)$ show that the definitions of Eqns. 156 and 157 lead to

$$\tilde{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(x) \exp(-ipx/\hbar)\,\mathrm{d}x$$
$$\phi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \tilde{\phi}(p) \exp(ipx/\hbar)\,\mathrm{d}p.$$

ANS: making the substitutions, and using

$$\phi(x) \triangleq f\left(x/\sqrt{2\pi\hbar}\right)$$
$$\tilde{\phi}(p) \triangleq \tilde{f}\left(p/\sqrt{2\pi\hbar}\right)$$

gives the desired result.

7.2.2

(a) We can resolve the identity $\hat{\mathbb{I}}$ into either the position basis:

$$\hat{\mathbb{I}} = \int_{-\infty}^{\infty} |x\rangle\langle x|\mathrm{d}x \tag{158}$$

or momentum basis:

$$\hat{\mathbb{I}} = \int_{-\infty}^{\infty} |p\rangle\langle p|\mathrm{d}p. \tag{159}$$

Define the ket $|\phi\rangle$ such that its projection into the position basis is $\phi(x)$, *i.e.*

$$\langle x|\phi\rangle \triangleq \phi(x). \tag{160}$$

For consistency we would like the projection of $|\phi\rangle$ into the momentum basis to be the Fourier transform of this:

$$\langle p|\phi\rangle = \tilde{\phi}(p) \,. \tag{161}$$

That is, we would like

$$\tilde{\phi}(p) = \mathrm{FT}\left[\phi(x)\right] \tag{162}$$
$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp\left(-ipx/\hbar\right)\phi(x)\,\mathrm{d}x. \tag{163}$$

By inserting a resolution of the identity in the position basis (Eq. 158) into Eq. 161 show that we require

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(-ipx/\hbar\right). \tag{164}$$

ANS:

$$\begin{aligned}\tilde{\phi}(p) &= \langle p|\phi\rangle \\ &= \int \langle p|x\rangle\langle x|\phi\rangle \mathrm{d}x \\ &= \int \langle p|x\rangle \phi(x)\,\mathrm{d}x\end{aligned}$$

therefore the result follows iff

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(-ipx/\hbar\right).$$

(b) We expect $\phi(x)$ to be the inverse Fourier transform (FT^{-1}) of $\tilde{\phi}(p)$, *i.e.*

$$\phi(x) = \mathrm{FT}^{-1}\left[\tilde{\phi}(p)\right] \tag{165}$$
$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp\left(ipx/\hbar\right)\tilde{\phi}(p)\,\mathrm{d}p. \tag{166}$$

Show that this implies

$$\left(\langle p|x\rangle\right)^{*} = \langle x|p\rangle. \tag{167}$$

ANS:

$$
\begin{aligned}
\phi(x) &= \langle x|\phi\rangle \\
&= \int \langle x|p\rangle\langle p|\phi\rangle \mathrm{d}p \\
&= \int \langle x|p\rangle\tilde{\phi}(p)\,\mathrm{d}p
\end{aligned}
$$

so the relation follows iff

$$
\begin{aligned}
\langle x|p\rangle &= \frac{1}{\sqrt{2\pi\hbar}}\exp(ipx/\hbar) \\
&= (\langle p|x\rangle)^{*}\,.
\end{aligned}
$$

Why is a relation of this form desirable?

ANS: $\langle x|p\rangle$ is a complex scalar, so $(\langle x|p\rangle)^{*} = \langle p|x\rangle$ in general. It is a requirement of the inner product.

(c) Since $|p\rangle$ is a momentum eigenstate, we expect $\langle x|p\rangle$ to be the wavefunction of a momentum eigenstate written in the position basis, *i.e.*

$$\hat{p}(\langle x|p\rangle) = -i\hbar\partial_x(\langle x|p\rangle) = p(\langle x|p\rangle)\,. \tag{168}$$

Check that this is indeed the case.

7.2.3

(a) The states $\{|x\rangle\}$ are orthonormal, *i.e.*

$$\langle x|x'\rangle = \delta(x-x') \tag{169}$$

where the Dirac delta function is defined by

$$\int_{-\infty}^{\infty}\delta(x-x')\,f(x')\,\mathrm{d}x' = f(x)\,. \tag{170}$$

Show that this implies the relation

$$2\pi\delta(x) = \frac{1}{\hbar}\int_{-\infty}^{\infty}\exp(ixp/\hbar)\,\mathrm{d}p. \tag{171}$$

ANS:

$$\begin{aligned}\delta\left(x-x'\right)=\langle x|x'\rangle &= \int \langle x|p\rangle\langle p|x'\rangle \mathrm{d}p \\ &= \frac{1}{2\pi\hbar}\int \exp\left(i\left(x-x'\right)p/\hbar\right)\mathrm{d}p \\ &= \int \exp\left(2\pi i\left(x-x'\right)p\right)\mathrm{d}p.\end{aligned}$$

(b) The states $\{|p\rangle\}$ are also orthonormal, *i.e.*

$$\langle p|p'\rangle = \delta\left(p-p'\right). \tag{172}$$

Show that this gives

$$2\pi\delta\left(p\right) = \frac{1}{\hbar}\int_{-\infty}^{\infty} \exp\left(ixp/\hbar\right)\mathrm{d}x.$$

ANS:

$$\begin{aligned}\delta\left(p-p'\right)=\langle p|p'\rangle &= \int \langle p|x\rangle\langle x|p'\rangle \mathrm{d}x \\ &= \frac{1}{2\pi\hbar}\int \exp\left(i\left(p'-p\right)x/\hbar\right)\mathrm{d}x.\end{aligned}$$

7.2.4

Using the forms

$$\mathrm{FT}\left[\phi\left(x\right)\right] = \int_{-\infty}^{\infty} \langle p|x\rangle\phi\left(x\right)\mathrm{d}x \tag{173}$$

$$\mathrm{FT}^{-1}\left[\tilde{\phi}\left(p\right)\right] = \int_{-\infty}^{\infty} \langle x|p\rangle\tilde{\phi}\left(p\right)\mathrm{d}p \tag{174}$$

and Eqs. 169 and 172 show that

$$\tilde{\phi}\left(p\right) = \mathrm{FT}\left[\mathrm{FT}^{-1}\left[\tilde{\phi}\left(p\right)\right]\right] \tag{175}$$

and

$$\phi\left(x\right) = \mathrm{FT}^{-1}\left[\mathrm{FT}\left[\phi\left(x\right)\right]\right]. \tag{176}$$

ANS:

$$
\begin{aligned}
\mathrm{FT}\left[\mathrm{FT}^{-1}\left[\tilde{\phi}(p)\right]\right] &= \int \mathrm{d}x \int \mathrm{d}p' \langle p|x\rangle\langle x|p'\rangle\tilde{\phi}(p') \\
&= \int \mathrm{d}p' \langle p| \left(\int \mathrm{d}x |x\rangle\langle x|\right) |p'\rangle\tilde{\phi}(p') \\
&= \int \mathrm{d}p' \langle p|p'\rangle\tilde{\phi}(p') \\
&= \int \mathrm{d}p' \delta(p-p')\,\tilde{\phi}(p') \\
&= \tilde{\phi}(p)\,.
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{FT}^{-1}\left[\mathrm{FT}\left[\phi(x)\right]\right] &= \int \mathrm{d}p \langle x|p\rangle \int \mathrm{d}x' \langle p|x'\rangle\phi(x') \\
&= \int \mathrm{d}x' \langle x| \left(\int \mathrm{d}p |p\rangle\langle p|\right) |x'\rangle\phi(x') \\
&= \int \mathrm{d}x' \langle x|x'\rangle\phi(x') \\
&= \int \mathrm{d}x' \delta(x-x')\,\phi(x') \\
&= \phi(x)\,.
\end{aligned}
$$

7.3 Justifying the differential operators

7.3.1

A function of an operator $\phi(\hat{x})$ can be defined by its Taylor series. Defining an arbitrary function $f(x)$ such that

$$\hat{x} f(x) = x f(x) \tag{177}$$

show that

$$[\phi(\hat{x}), \hat{p}]\, f(x) = i\hbar \frac{\partial \phi(x)}{\partial x} f(x)\,. \tag{178}$$

ANS:

This was done in video V6.1 Ehrenfest's theorem. By definition we have

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

and we can show

$$[\hat{x}^n, \hat{p}] = ni\hbar\hat{x}^{n-1}$$

by repeatedly pulling the $\hat{p}$ operator through the $\hat{x}$; for example,

$$\begin{aligned}
\left[\hat{x}^2, \hat{p}\right] &= \hat{x}^2\hat{p} - \hat{p}\hat{x}^2 \\
&= \hat{x}^2\hat{p} - (\hat{p}\hat{x})\,\hat{x} \\
&= \hat{x}^2\hat{p} - (\hat{x}\hat{p} - [\hat{x}, \hat{p}])\,\hat{x} \\
&= \hat{x}^2\hat{p} - \hat{x}\hat{p}\hat{x} + i\hbar\hat{x} \\
&= \hat{x}^2\hat{p} - \hat{x}\,(\hat{p}\hat{x}) + i\hbar\hat{x} \\
&= \hat{x}^2\hat{p} - \hat{x}\,(\hat{x}\hat{p} - [\hat{x}, \hat{p}]) + i\hbar\hat{x} \\
&= \hat{x}^2\hat{p} - \hat{x}^2\hat{p} + 2i\hbar\hat{x} \\
&= 2i\hbar\hat{x}.
\end{aligned}$$

The same reasoning leads to the above result. Since $\phi(\hat{x})$ is defined by its Taylor series, which is a sum of powers of $\hat{x}$, and

$$[\hat{x}^n, \hat{p}] = ni\hbar\hat{x}^{n-1}$$

is a derivative of power $\hat{x}^n$ multiplied by $i\hbar$, it follows that

$$[\phi(\hat{x}), \hat{p}]\, f(x) = i\hbar\frac{\partial\phi(x)}{\partial x} f(x)\,.$$

The reason for acting on an arbitrary function $f(x)$ is just that the more general expression

$$[\phi(\hat{x}), \hat{p}] = i\hbar\frac{\partial\phi(\hat{x})}{\partial\hat{x}}$$

requires the derivative with respect to an operator to be defined; it's hopefully clear what this would mean, but the definition above does not require it.

7.3.2

By expanding the commutator (or otherwise) explain why it is natural to assign $\hat{p}f(x) = -i\hbar\partial_x f(x)$.

ANS:

$$\hat{p}\phi(\hat{x}) f(x) = \phi(\hat{x}) \hat{p} f(x) - i\hbar \frac{\partial \phi(x)}{\partial x} f(x) . \tag{179}$$

7.4 Hermiticity of differential operators

7.4.1

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

ANS:

$$\int_{-\infty}^{\infty} \varphi(x)^* \left(\hat{A}^\dagger \psi(x)\right) \mathrm{d}x \triangleq \int_{-\infty}^{\infty} \left(\hat{A}\varphi(x)\right)^* \psi(x) \, \mathrm{d}x \;\forall \varphi, \psi.$$

7.4.2

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

(a) x

(b) ∂_x

(c) $-i\hbar\partial_x$

(d) ∂_x^2

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

(f) ∇

ANS:

all Hermitian except $(\partial_x)^\dagger = -\partial_x$ and $\nabla^\dagger = \nabla$.

8 The quantum harmonic oscillator

Bring solutions along to the class at 10am on 23/11/20.

Questions marked # are beyond the syllabus. We may discuss them in the class if there is time.

Attempt all questions. Feel free to discuss with friends. Don't worry if you cannot answer a question fully as you will discuss the solutions in the class.

8.0 Videos

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8.1 Solution using Hermite polynomials

The Hamiltonian for the quantum harmonic oscillator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2. \tag{180}$$

8.1.1

Working in the position basis, define

$$x = \alpha y \tag{181}$$

for suitable α to show that the TISE can be written

$$-\frac{1}{2}\frac{\mathrm{d}^2\phi_n(y)}{\mathrm{d}y^2} + \frac{1}{2}y^2\phi_n(y) = \epsilon_n\phi_n(y) \tag{182}$$

and state an expression for ϵ_n.

ANS:

In the position basis,

$$\left(-\frac{\hbar^2}{2m}\partial_x^2 + \frac{1}{2}m\omega^2x^2\right)\varphi(x) = E\varphi(x).$$

Rescale:

$$\left(-\frac{\hbar^2}{2m\alpha^2}\partial_y^2 + \frac{1}{2}m\omega^2\alpha^2y^2\right)\varphi(\alpha y) = E\varphi(\alpha y).$$

Let

$$\phi(y) = \varphi(\alpha y).$$

We'd like the two terms in parentheses to have the same coefficient, i.e.

$$\frac{\hbar^2}{2m\alpha^2} = \frac{m\omega^2\alpha^2}{2}$$

so choose

$$\alpha = \sqrt{\frac{\hbar}{m\omega}}$$

giving

$$\frac{1}{2}\hbar\omega\left(-\partial_y^2 + y^2\right)\phi(y) = E\phi(y)$$

or

$$\frac{1}{2}\left(-\partial_y^2 + y^2\right)\phi(y) = \epsilon\phi(y)$$

with

$$\epsilon = \frac{E}{\hbar\omega}.$$

8.1.2

Using the ansatz

$$\phi_n(y) = H_n(y)\exp\left(-y^2/2\right) \tag{183}$$

show that Eq. 182 can be rewritten as Hermite's equation

$$H_n(y)'' - 2yH_n(y)' + (2\epsilon - 1)H_n(y) = 0. \tag{184}$$

ANS:

$$\begin{aligned}
\phi' &= H'\exp\left(-y^2/2\right) - y\phi \\
\phi'' &= H''\exp\left(-y^2/2\right) - yH'\exp\left(-y^2/2\right) - \phi - y\phi' \\
&= H''\exp\left(-y^2/2\right) - 2yH'\exp\left(-y^2/2\right) - \phi + y^2\phi
\end{aligned}$$

therefore

$$
\begin{aligned}
-\phi'' + y^2\phi &= 2\epsilon\phi \\
&\downarrow \\
H'' \exp\left(-y^2/2\right) - 2yH' \exp\left(-y^2/2\right) + (2\epsilon - 1)\,\phi &= 0 \\
H'' - 2yH' + (2\epsilon - 1)\,H &= 0.
\end{aligned}
$$

8.1.3

The solutions are 'Hermite polynomials', defined by:

$$H_0 = 1 \tag{185}$$

$$H_{n\geq 1}(y) = (-1)^n \exp\left(y^2\right) \frac{\mathrm{d}^n}{\mathrm{d}y^n} \exp\left(-y^2\right). \tag{186}$$

Find the first four Hermite polynomials explicitly, and sketch them. Therefore, sketch the first four energy eigenstates of the harmonic oscillator $\phi_n(x)$.

ANS:

$$
\begin{aligned}
H_0(y) &= 1 \\
H_1(y) &= 2y \\
H_2(y) &= \exp\left(y^2\right) \frac{\mathrm{d}^2}{\mathrm{d}y^2} \exp\left(-y^2\right) \\
&= \exp\left(y^2\right) \left(\frac{\mathrm{d}}{\mathrm{d}y} \left(-2y \exp\left(-y^2\right)\right) \right) \\
&= -2 + 4y^2 \\
H_3(y) &= -\exp\left(y^2\right) \left(\frac{\mathrm{d}}{\mathrm{d}y} \left(\left(-2 + 4y^2\right) \exp\left(-y^2\right) \right) \right) \\
&= 2y\left(-2 + 4y^2\right) - 8y \\
&= -12y + 8y^3
\end{aligned}
$$

the sketches are straightforward, noting that $\phi_n(y) = H_n(y) \exp\left(-y^2/2\right)$.

8.2 Ladder operators

8.2.1

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

$$\hat{H} = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}y^2} + \frac{1}{2}y^2. \tag{187}$$

Show this can be rewritten as

$$\hat{H} = \hat{a}^\dagger\hat{a} + \frac{1}{2}\hat{\mathbb{I}} \tag{188}$$

where the lowering operator is

$$\hat{a} = \frac{1}{\sqrt{2}}\left(y + \frac{\mathrm{d}}{\mathrm{d}y}\right) \tag{189}$$

and the raising operator is

$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(y - \frac{\mathrm{d}}{\mathrm{d}y}\right) \tag{190}$$

(collectively they are known as ladder operators).

ANS:

$$\begin{aligned}\hat{a}^\dagger\hat{a} &= \frac{1}{2}\left(y - \frac{\mathrm{d}}{\mathrm{d}y}\right)\left(y + \frac{\mathrm{d}}{\mathrm{d}y}\right)\\ &= \frac{1}{2}\left(y^2 - \frac{\mathrm{d}^2}{\mathrm{d}y^2} + y\frac{\mathrm{d}}{\mathrm{d}y} - 1 - y\frac{\mathrm{d}}{\mathrm{d}y}\right)\\ &= \frac{1}{2}\left(y^2 - \frac{\mathrm{d}^2}{\mathrm{d}y^2} - 1\right).\end{aligned}$$

8.2.2

Show, using the definition of the Hermitian conjugate for differential operators, that $\hat{a}^\dagger$ is the Hermitian conjugate of $\hat{a}$.

ANS:

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

so we need to show that

$$\int_{-\infty}^{\infty} \varphi(y)^* \left(\hat{a}^\dagger \psi(y)\right) \mathrm{d}y \triangleq \int_{-\infty}^{\infty} \left(\hat{a}\varphi(y)\right)^* \psi(y)\,\mathrm{d}y.$$

From the right-hand side:

$$\begin{aligned}\int_{-\infty}^{\infty} \left(\hat{a}\varphi(y)\right)^* \psi(y)\,\mathrm{d}y &= \frac{1}{\sqrt{2}}\int_{-\infty}^{\infty}\left(y\varphi^*(y) + \frac{\mathrm{d}}{\mathrm{d}y}\varphi^*(y)\right)\psi(y)\,\mathrm{d}y \\ &= \frac{1}{\sqrt{2}}\int_{-\infty}^{\infty}\left(y\varphi^*(y)\psi(y) + \psi(y)\frac{\mathrm{d}}{\mathrm{d}y}\right)\mathrm{d}y \\ &\downarrow \text{integration by parts} \\ &= \frac{1}{\sqrt{2}}\int_{-\infty}^{\infty}\left(y\varphi^*(y)\psi(y) - \varphi^*(y)\frac{\mathrm{d}\psi(y)}{\mathrm{d}y}\right)\mathrm{d}y\end{aligned}$$

(the boundary term vanishes as φ and ψ are assumed to be normalisable and therefore vanish at infinity) and so

$$\int_{-\infty}^{\infty} \left(\hat{a}\varphi(y)\right)^* \psi(y)\,\mathrm{d}y = \int_{-\infty}^{\infty} \varphi^*(y)\frac{1}{\sqrt{2}}\left(y - \frac{\mathrm{d}}{\mathrm{d}y}\right)\psi(y)\,\mathrm{d}y$$

telling us that

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

as required.

8.2.3

Show that

$$\left[\hat{a}, \hat{a}^\dagger\right] = \hat{\mathbb{I}}. \tag{191}$$

ANS:

$$\begin{aligned}
\hat{a}\hat{a}^{\dagger} f &= \frac{1}{2}\left(y + \frac{\partial}{\partial y}\right)\left(y - \frac{\partial}{\partial y}\right) f \\
&= \frac{1}{2}\left(y + \frac{\partial}{\partial y}\right)(yf - f') \\
&= \frac{1}{2}\left(y^2 f - yf' + f + yf' - f''\right) \\
&= \frac{1}{2}\left(y^2 f + f - f''\right)
\end{aligned}$$

and

$$\begin{aligned}
\hat{a}^{\dagger}\hat{a} f &= \frac{1}{2}\left(y - \frac{\partial}{\partial y}\right)\left(y + \frac{\partial}{\partial y}\right) f \\
&= \frac{1}{2}\left(y - \frac{\partial}{\partial y}\right)(yf + f') \\
&= \frac{1}{2}\left(y^2 f + yf' - f - yf' - f''\right) \\
&= \frac{1}{2}\left(y^2 f - f - f''\right).
\end{aligned}$$

Therefore

$$\hat{a}\hat{a}^{\dagger} f - \hat{a}^{\dagger}\hat{a} f = f.$$

We can rewrite this as

$$\left[\hat{a}, \hat{a}^{\dagger}\right] f = f$$

and since f is arbitrary this holds at the operator level:

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

8.2.4

Show that

$$\left[\hat{a}^{\dagger}, \hat{H}\right] = -\hat{a}^{\dagger}. \tag{192}$$

ANS:

$$\begin{aligned}\left[\hat{a}^\dagger, \hat{H}\right] &= \hat{a}^\dagger \hat{H} - \hat{H}\hat{a}^\dagger \\ &= \hat{a}^\dagger \hat{a}^\dagger \hat{a} + \frac{1}{2}\hat{a}^\dagger - \left(\hat{a}^\dagger \hat{a} \hat{a}^\dagger + \frac{1}{2}\hat{a}^\dagger\right) \\ &= \hat{a}^\dagger \hat{a}^\dagger \hat{a} - \hat{a}^\dagger \hat{a} \hat{a}^\dagger \\ &= \hat{a}^\dagger \left[\hat{a}^\dagger, \hat{a}\right] \\ &= -\hat{a}^\dagger .\end{aligned}$$

8.2.5

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

$$\hat{H}\phi_n(y) = \epsilon_n \phi_n(y) \tag{193}$$

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

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

ANS:

$$\begin{aligned}\hat{a}^\dagger \hat{H}\phi(y) &= \epsilon \hat{a}^\dagger \phi(y) \\ \left(\hat{H}\hat{a}^\dagger + \left[\hat{a}^\dagger, \hat{H}\right]\right)\phi(y) &= \epsilon \hat{a}^\dagger \phi(y) \\ \left(\hat{H}\hat{a}^\dagger - \hat{a}^\dagger\right)\phi(y) &= \epsilon \hat{a}^\dagger \phi(y) \\ \hat{H}\hat{a}^\dagger \phi(y) &= (\epsilon + 1)\hat{a}^\dagger \phi(y).\end{aligned}$$

8.2.6

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

ANS:

Given any energy eigenstate ϕ_n with energy eigenvalue ϵ_n, we can act with $\hat{a}^\dagger$ to obtain a new energy eigenstate whose energy eigenvalue is $\epsilon_n + 1$. Therefore there are energy eigenstates with eigenvalues $\epsilon_n + m$ for arbitrary positive integers m.

8.2.7

Explain why it must be the case that

$$\int_{-\infty}^{\infty} |\hat{a}\phi_n(y)|^2 \,\mathrm{d}y \geq 0. \tag{194}$$

Hence argue that there is a lowest rung to the ladder of energies.

ANS:

$\hat{a}\phi_n(y)$ is either proportional to ϕ_{n-1}, or $\hat{a}\phi_n = 0$. This is straightforward to see in Dirac notation, as shown in the notes; the only tricky point in the present case is why $\hat{a}\phi = 0$ is legitimate. I'd say the best answer is that if we think of all possible things $\hat{a}\phi$ can be, given that the commutation relations have told us $\hat{H}(\hat{a}\phi_n) = (\epsilon - 1)(\hat{a}\phi_n)$, these are the only two possibilities, so let's consider them both. In Dirac notation we're reminded instantly that $\hat{a}|n\rangle$ is a state in a Hilbert space, requiring that $\|\hat{a}|n\rangle\| \geq 0$ with equality iff $\hat{a}|n\rangle = 0$.

For any normalised energy eigenstate ϕ_n we have that

$$\int_{-\infty}^{\infty} |\phi_n(y)|^2 \,\mathrm{d}y = 1.$$

For the cases that

$$\hat{a}\phi_n \propto \phi_{n-1}$$

since it's only a proportionality we can only say that

$$\hat{a}\phi_n = c\phi_{n-1}$$

where c is a possibly complex constant. Still, since ϕ_{n-1} is still normalised by definition, we know that

$$\begin{aligned}\int_{-\infty}^{\infty} |\hat{a}\phi_n(y)|^2 \,\mathrm{d}y &= |c|^2 \int_{-\infty}^{\infty} |\phi_{n-1}(y)|^2 \,\mathrm{d}y \\ &= |c|^2 > 0.\end{aligned}$$

For the equality we must instead have the case $\hat{a}\phi_0 = 0$.

Since

$$\int_{-\infty}^{\infty} |\hat{a}\phi_n(y)|^2 \,\mathrm{d}y \geq 0$$

we have

$$\begin{aligned}0 \leq & \int_{-\infty}^{\infty} \phi_n^*(y)\, \hat{a}^\dagger \hat{a} \phi_n(y)\, \mathrm{d}y \\ = & \int_{-\infty}^{\infty} \phi_n^*(y) \left(\hat{H} - \frac{1}{2}\right) \phi_n(y)\, \mathrm{d}y \\ = & \left(\epsilon_n - \frac{1}{2}\right) \int_{-\infty}^{\infty} \phi_n^*(y)\, \phi_n(y)\, \mathrm{d}y \\ = & \epsilon_n - \frac{1}{2}.\end{aligned}$$

Therefore

$$\epsilon_n \geq \frac{1}{2}$$

and there is a lowest rung to the ladder.

8.2.8

The eigenstate on the lowest rung must obey this condition:

$$\hat{a}\phi_0(y) = 0. \tag{195}$$

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

ANS:

$$\begin{aligned}\frac{1}{\sqrt{2}} \left(y + \frac{\mathrm{d}}{\mathrm{d}y}\right) \phi_0(y) = 0 \\ \downarrow \\ \frac{\mathrm{d}\phi_0}{\mathrm{d}y} &= -y\phi_0 \\ \int \frac{\mathrm{d}\phi_0}{\phi_0} &= -\int y\mathrm{d}y \\ \phi_0(y) &= A \exp\left(-y^2/2\right)\end{aligned}$$

and normalise:

$$\int_{-\infty}^{\infty} |\phi_0|^2 \, \mathrm{d}y = 1 = |A|^2 \int_{-\infty}^{\infty} \exp\left(-y^2\right) \mathrm{d}y$$
$$= \pi \, |A|^2$$

so

$$\phi_0 \left(y\right) = \frac{1}{\sqrt{\pi}} \exp\left(-y^2/2\right).$$

Then we use

$$\hat{H}\phi_0 = \epsilon_0 \phi_0$$
$$\left(\hat{a}^\dagger \hat{a} + \frac{1}{2}\right) \phi_0 = \frac{1}{2}\phi_0$$

to find $\epsilon_0 = 1/2$.

8.2.9

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

ANS:

$$\phi_1 \left(y\right) = A_1 \hat{a}^\dagger \phi_0 \left(y\right)$$
$$= A_1 \frac{1}{\sqrt{2\pi}} \left(y - \frac{\mathrm{d}}{\mathrm{d}y}\right) \exp\left(-y^2/2\right)$$
$$= A_1 \sqrt{\frac{2}{\pi}} y \exp\left(-y^2/2\right)$$

normalisation:

$$\int |\phi_1|^2 \, \mathrm{d}y = 1 = |A_1|^2 \, \frac{2}{\pi} \int_{-\infty}^{\infty} y^2 \exp\left(-y^2\right) \mathrm{d}y$$
$$= |A_1|^2 \, \frac{1}{\sqrt{\pi}}$$

so

$$\phi_1(y) = 2^{1/2}\pi^{1/4} y \exp\left(-y^2/2\right)$$

and

$$\hat{H}\phi_1 = \epsilon_1\phi_1$$
$$\left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}y^2} + \frac{1}{2}y^2\right)\phi_1 = \frac{3}{2}\phi_1$$

$$\epsilon_1 = 3/2.$$

8.2.10

Explain why

$$\hat{a}^\dagger \hat{a}\phi_n \propto \phi_n. \tag{196}$$

By multiplying both sides by ϕ_n^* and integrating over all y, show that the constant of proportionality is n.

ANS:

Since

$$\hat{a}\phi_n \propto \phi_{n-1}$$

and

$$\hat{a}^\dagger\phi_n \propto \phi_{n+1}$$

the result follows.

To find the constant of proportionality, use that

$$\begin{aligned}
\hat{a}^\dagger \hat{a}\phi_n &= A\phi_n \\
\int \phi_n^* \hat{a}^\dagger \hat{a}\phi_n &= A \int \phi_n^* \phi_n \mathrm{d}y \\
\int \phi_n^* \left(\hat{H} - 1/2\right) \phi_n &= A \\
\int \phi_n^* \left(\epsilon_n - 1/2\right) \phi_n &= A \\
\epsilon_n - 1/2 &= A \\
n &= A
\end{aligned}$$

i.e.

$$\hat{a}^\dagger \hat{a}\phi_n = n\phi_n.$$

8.2.11

Show that

$$\hat{a}\phi_n = \sqrt{n}\phi_{n-1}. \tag{197}$$

ANS:

we know that

$$\hat{a}\phi_n = B\phi_{n-1}.$$

To find the constant of proportionality, take the modulus square of both sides, and integrate:

$$\begin{aligned}
\int |\hat{a}\phi_n|^2 \mathrm{d}y &= |B|^2 \int |\phi_{n-1}|^2 \mathrm{d}y \\
\int \phi_n^* \hat{a}^\dagger \hat{a}\phi_n \mathrm{d}y &= |B|^2 \\
\int \phi_n^* \left(\hat{H} - 1/2\right) \phi_n \mathrm{d}y &= |B|^2 \\
n &= |B|^2
\end{aligned}$$

so

$$\hat{a}\phi_n = \sqrt{n}\phi_{n-1}$$

up to a global phase.

8.2.12

Show that

$$\hat{a}^\dagger\phi_n = \sqrt{n+1}\phi_{n+1}. \tag{198}$$

ANS:

$$\begin{aligned}
\hat{a}^\dagger\phi_n &= C\phi_{n+1} \\
\int \left|\hat{a}^\dagger\phi_n\right|^2 \mathrm{d}y &= |C|^2 \int |\phi_{n+1}|^2 \mathrm{d}y \\
\int \phi_n^* \hat{a}\hat{a}^\dagger \phi_n \mathrm{d}y &= |C|^2 \\
\int \phi_n^* \left(\hat{a}^\dagger\hat{a} - \left[\hat{a}^\dagger, \hat{a}\right]\right) \phi_n \mathrm{d}y &= |C|^2 \\
\int \phi_n^* \left(\hat{H} - 1/2 + 1\right) \phi_n \mathrm{d}y &= |C|^2 \\
n + 1 &= |C|^2
\end{aligned}$$

therefore

$$\hat{a}^\dagger\phi_n = \sqrt{n+1}\phi_{n+1}$$

up to a global phase.

8.2.13

Hence explain why we can write any normalised eigenstate of the harmonic oscillator as

$$\phi_n(y) = \frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n \phi_0(y). \tag{199}$$

ANS:

$$\begin{aligned}
&\left(\hat{a}^\dagger\right)^n \phi_0 \\
&= \left(\hat{a}^\dagger\right)^{n-1} \phi_1 \\
&= \left(\hat{a}^\dagger\right)^{n-2} \sqrt{2\cdot 1}\phi_2 \\
&= \left(\hat{a}^\dagger\right)^{n-3} \sqrt{3\cdot 2\cdot 1}\phi_3 \\
&\vdots \\
&= \sqrt{n!}\phi_n.
\end{aligned}$$

8.3 Ladder operators redone

In this question we will redo question 8.2 in a basis-independent manner, using just the canonical commutation relations and Dirac notation. We will not rescale the variables, partly because this is less necessary and partly because it's good to be familiar with different ways of approaching the problem. Check you understand how each result relates to the corresponding result in 8.2.

8.3.1

The Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2. \tag{200}$$

Show this can be rewritten as

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\hat{\mathbb{I}}\right) \tag{201}$$

where the lowering operator is

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) \tag{202}$$

and the raising operator is

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right) \tag{203}$$

(collectively they are known as ladder operators).

ANS:

$$\begin{aligned}
\hat{a}^\dagger\hat{a} &= \frac{m\omega}{2\hbar}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) \\
&= \frac{m\omega}{2\hbar}\left(\hat{x}^2 + \frac{1}{m^2\omega^2}\hat{p}^2 - \frac{i}{m\omega}\hat{p}\hat{x} + \frac{i}{m\omega}\hat{x}\hat{p}\right) \\
&= \frac{m\omega}{2\hbar}\left(\hat{x}^2 + \frac{1}{m^2\omega^2}\hat{p}^2 + \frac{i}{m\omega}\left[\hat{x},\hat{p}\right]\right) \\
&= \frac{m\omega}{2\hbar}\left(\hat{x}^2 + \frac{1}{m^2\omega^2}\hat{p}^2 + \frac{i}{m\omega}i\hbar\hat{\mathbb{I}}\right) \\
&= \frac{m\omega}{2\hbar}\left(\hat{x}^2 + \frac{1}{m^2\omega^2}\hat{p}^2 - \frac{\hbar}{m\omega}\hat{\mathbb{I}}\right)
\end{aligned}$$

therefore

$$\hbar\omega\hat{a}^\dagger\hat{a} = \frac{m\omega^2}{2}\hat{x}^2 + \frac{1}{2m}\hat{p}^2 - \frac{\hbar\omega}{2}\hat{\mathbb{I}}$$

and so

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

as required.

8.3.2

Show that $\hat{a}^\dagger$ is the Hermitian conjugate of $\hat{a}$.

ANS:

$$\begin{aligned}
\hat{a} &= \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) \\
&\downarrow \\
\hat{a}^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}^\dagger - \frac{i}{m\omega}\hat{p}^\dagger\right) \\
\hat{a}^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)
\end{aligned}$$

where the last line follows as $\hat{x}$ and $\hat{p}$ are Hermitian (as they correspond to observables).

8.3.3

Show that

$$\left[\hat{a}, \hat{a}^\dagger\right] = \hat{\mathbb{I}}. \tag{204}$$

ANS:

$$\begin{aligned}
\left[\hat{a}, \hat{a}^\dagger\right] &= \left[\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right), \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)\right] \\
&= \frac{m\omega}{2\hbar}\left[\hat{x} + \frac{i}{m\omega}\hat{p}, \hat{x} - \frac{i}{m\omega}\hat{p}\right] \\
&= -i\frac{1}{\hbar}\left[\hat{x}, \hat{p}\right] \\
&= -i\frac{1}{\hbar}i\hbar\hat{\mathbb{I}} \\
&= \hat{\mathbb{I}}.
\end{aligned}$$

8.3.4

Show that

$$\left[\hat{a}^\dagger, \hat{H}\right] = -\hbar\omega\hat{a}^\dagger. \tag{205}$$

ANS:

$$\begin{aligned}
\left[\hat{a}^\dagger, \hat{H}\right] &= \hat{a}^\dagger\hat{H} - \hat{H}\hat{a}^\dagger \\
&= \hbar\omega\left\{\hat{a}^\dagger\hat{a}^\dagger\hat{a} + \frac{1}{2}\hat{a}^\dagger - \left(\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \frac{1}{2}\hat{a}^\dagger\right)\right\} \\
&= \hbar\omega\left\{\hat{a}^\dagger\hat{a}^\dagger\hat{a} - \hat{a}^\dagger\hat{a}\hat{a}^\dagger\right\} \\
&= \hbar\omega\left\{\hat{a}^\dagger\left[\hat{a}^\dagger, \hat{a}\right]\right\} \\
&= -\hbar\omega\hat{a}^\dagger.
\end{aligned}$$

8.3.5

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

$$\hat{H}|n\rangle = E_n|n\rangle \tag{206}$$

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

$$\hat{H}\left(\hat{a}^\dagger|n\rangle\right) = \left(E_n + \hbar\omega\right)\left(\hat{a}^\dagger|n\rangle\right).$$

ANS:

$$
\begin{aligned}
\hat{a}^\dagger \hat{H}|n\rangle &= E_n \hat{a}^\dagger |n\rangle \\
\left(\hat{H}\hat{a}^\dagger + \left[\hat{a}^\dagger, \hat{H}\right]\right)|n\rangle &= E_n \hat{a}^\dagger |n\rangle \\
\left(\hat{H}\hat{a}^\dagger - \hbar\omega\hat{a}^\dagger\right)|n\rangle &= E_n \hat{a}^\dagger |n\rangle \\
\hat{H}\hat{a}^\dagger|n\rangle &= \left(E_n + \hbar\omega\right)\hat{a}^\dagger|n\rangle.
\end{aligned}
$$

8.3.6

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

ANS:

Given any energy eigenstate $|n\rangle$ with energy eigenvalue E_n, we can act with $\hat{a}^\dagger$ to obtain a new energy eigenstate whose energy eigenvalue is $E_n + \hbar\omega$. Therefore there are energy eigenstates with eigenvalues $E_n + m\hbar\omega$ for arbitrary positive integers m.

8.3.7

Explain why it must be the case that

$$\left\|\hat{a}|n\rangle\right\|^2 \geq 0. \tag{207}$$

Hence argue that there is a lowest rung to the ladder of energies.

ANS:

$|n\rangle$ is a state in a Hilbert space, and so is $\hat{a}|n\rangle$. A Hilbert space is just a linear vector space with an inner product. One of the axioms of inner product spaces is that the norm of any vector $|v\rangle$ has the property $\left\||v\rangle\right\|^2 \geq 0$, where $\left\||v\rangle\right\|^2 = 0$ iff $|v\rangle = 0$.

We know the norm is defined as

$$\left\||v\rangle\right\|^2 = \langle v|v\rangle.$$

Therefore

$$
\begin{aligned}
\langle n|\hat{a}^\dagger\hat{a}|n\rangle &\geq 0 \\
\langle n|\frac{1}{\hbar\omega}\hat{H} - \frac{1}{2}\hat{\mathbb{I}}|n\rangle &\geq 0 \\
E_n &\geq \frac{\hbar\omega}{2}
\end{aligned}
$$

and since there is a lowest energy eigenvalue (the values step by $\hbar\omega$) there is a lowest energy eigenstate.

8.3.8

The eigenstate on the lowest rung, $|0\rangle$ (just a state labelled 0, not the number zero!), must obey this condition:

$$\hat{a}|0\rangle = 0. \tag{208}$$

Use this equation to solve for the normalised eigenstate $\langle x|0\rangle = \varphi_0(x)$ and the corresponding energy eigenvalue E_0. Here we do need to work in the position basis.

ANS:

$$\begin{aligned}
\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)\varphi_0(x) &= 0 \\
\sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{\hbar}{m\omega}\partial_x\right)\varphi_0(x) &= 0 \\
\frac{\mathrm{d}\varphi_0}{\mathrm{d}x} &= -x\frac{m\omega}{\hbar}\varphi_0 \\
\int \frac{\mathrm{d}\varphi_0}{\varphi_0} &= -\frac{m\omega}{\hbar}\int x\mathrm{d}x \\
\varphi_0(x) &= A\exp\left(-m\omega x^2/2\hbar\right)
\end{aligned}$$

and normalise:

$$\begin{aligned}
\int_{-\infty}^{\infty} |\varphi_0|^2\,\mathrm{d}x = 1 &= |A|^2\int_{-\infty}^{\infty}\exp\left(-m\omega x^2/\hbar\right)\mathrm{d}x \\
&= |A|^2\sqrt{\frac{\hbar\pi}{m\omega}}
\end{aligned}$$

so

$$\phi_0(y) = \sqrt{\frac{m\omega}{\pi\hbar}}\exp\left(-m\omega x^2/2\hbar\right).$$

Then we use

$$\hat{H}\varphi_0(x) = E_0\varphi_0(x)$$
$$\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\varphi_0(x) = \hbar\omega\frac{1}{2}\varphi_0(x)$$

to find $E_0 = \hbar\omega/2$.

8.3.9

Find the normalised first excited state (in the position basis) and the corresponding energy eigenvalue.

ANS:

$$\begin{aligned}\varphi_1(x) &= A_1\hat{a}^\dagger\varphi_0(x)\\ &= A_1\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)\sqrt{\frac{m\omega}{\pi\hbar}}\exp\left(-m\omega x^2/2\hbar\right)\\ &= A_1\frac{m\omega}{\hbar}\frac{1}{\sqrt{2\pi}}\left(x - \frac{\hbar}{m\omega}\partial_x\right)\exp\left(-m\omega x^2/2\hbar\right)\\ &= A_1\frac{m\omega}{\hbar}\sqrt{\frac{2}{\pi}}x\exp\left(-m\omega x^2/2\hbar\right)\end{aligned}$$

normalisation:

$$\begin{aligned}\int|\varphi_1|^2\,\mathrm{d}x = 1 &= |A_1|^2\left(\frac{m\omega}{\hbar}\right)^2\frac{2}{\pi}\int_{-\infty}^{\infty}x^2\exp\left(-m\omega x^2/\hbar\right)\mathrm{d}x\\ &= |A_1|^2\left(\frac{m\omega}{\hbar}\right)^2\frac{2}{\pi}\frac{1}{2}\sqrt{\frac{\pi}{(m\omega/\hbar)^3}}\\ 1 &= |A_1|^2\sqrt{\frac{m\omega}{\pi\hbar}}\end{aligned}$$

so

$$\varphi_1(x) = \sqrt{2}\frac{m^{3/4}\omega^{3/4}}{\hbar^{3/4}\pi^{1/4}}x\exp\left(-m\omega x^2/2\hbar\right).$$

The energy eigenvalue we already know is $E_1 = E_0 + \hbar\omega = 3\hbar\omega/2$.

8.3.10

Explain why

$$\hat{a}^\dagger \hat{a}|n\rangle \propto |n\rangle. \tag{209}$$

Acting from the left with $\langle n|$ show that the constant of proportionality is n.

ANS:

Since

$$\hat{a}|n\rangle \propto |n-1\rangle$$

and

$$\hat{a}^\dagger|n\rangle \propto |n+1\rangle$$

the result follows.

To find the constant of proportionality, use that

$$\begin{aligned}
\hat{a}^\dagger \hat{a}|n\rangle &= A|n\rangle \\
\langle n|\hat{a}^\dagger \hat{a}|n\rangle &= A\langle n|n\rangle \\
\langle n|\frac{1}{\hbar\omega}\hat{H} - 1/2|n\rangle &= A \\
n &= A.
\end{aligned}$$

i.e.

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

8.3.11

Show that

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle. \tag{210}$$

ANS:

we know that

$$\hat{a}|n\rangle = B|n-1\rangle.$$

To find the constant of proportionality B, note that we're just finding the length of the vector $\hat{a}|n\rangle \parallel |n-1\rangle$, given that both $|n\rangle$ and $|n-1\rangle$ are by definition length 1 (normalised).

$$\begin{aligned} \| \hat{a}|n\rangle \|^2 &= |B|^2 \, \| |n-1\rangle \|^2 \\ \langle n|\hat{a}^\dagger \hat{a}|n\rangle &= |B|^2 \, \langle n-1|n-1\rangle \\ \langle n|\frac{1}{\hbar\omega}\hat{H} - 1/2|n\rangle &= |B|^2 \\ n &= |B|^2 \end{aligned}$$

so

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$$

up to a global phase.

8.3.12

Show that

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{211}$$

ANS:

$$\begin{aligned} \left\| \hat{a}^\dagger|n\rangle \right\|^2 &= |C|^2 \, \| |n+1\rangle \|^2 \\ \langle n|\hat{a}\hat{a}^\dagger|n\rangle &= |C|^2 \, \langle n+1|n+1\rangle \\ \langle n|\hat{a}^\dagger\hat{a} + \left[\hat{a}, \hat{a}^\dagger\right]|n\rangle &= |C|^2 \, \langle n+1|n+1\rangle \\ \langle n|\frac{1}{\hbar\omega}\hat{H} - 1/2 + 1|n\rangle &= |C|^2 \\ n+1 &= |C|^2 \end{aligned}$$

therefore

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

up to a global phase.

8.3.13

Hence explain why we can write any normalised eigenstate of the harmonic oscillator as

$$|n\rangle = \frac{1}{\sqrt{n!}} \left(\hat{a}^{\dagger}\right)^{n} |0\rangle. \tag{212}$$

ANS:

$$\begin{aligned} &\left(\hat{a}^{\dagger}\right)^{n} |0\rangle \\ =& \left(\hat{a}^{\dagger}\right)^{n-1} |1\rangle \\ =& \left(\hat{a}^{\dagger}\right)^{n-2} \sqrt{2 \cdot 1}|2\rangle \\ =& \left(\hat{a}^{\dagger}\right)^{n-3} \sqrt{3 \cdot 2 \cdot 1}|3\rangle \\ &\vdots \\ =& \sqrt{n!}|n\rangle. \end{aligned}$$

8.4 Second quantisation

Explain what is meant by second quantisation.

ANS:

Take-home point: first quantisation is the process of describing particles as waves; second quantisation is the process of describing waves as particles.

The state $|n\rangle$ can be thought of as the n^{th} excited state of the harmonic oscillator. In first-quantised language, $\langle x|n(t)\rangle = \psi_n(x,t)$; this is a stationary state with energy $(n+1/2)\hbar\omega$. But since this is equal to $\frac{1}{\sqrt{n!}}\left(\hat{a}^{\dagger}\right)^{n}|0\rangle$ it can equally well be thought of as n independent bosonic particles, each with energy $\hbar\omega$, sat in the harmonic potential. The fact that the total energy is not $n\hbar\omega$, but instead $(n+1/2)\hbar\omega$, is due to the ‘vacuum’ (absence of particles, state $|0\rangle$ itself) having an energy. This is the ‘zero point energy’.

9 The Schrödinger equation in three dimensions

Bring solutions along to the class at 10am on 30/11/20.

Questions marked # are beyond the syllabus. We may discuss them in the class if there is time. Attempt all questions. Feel free to discuss with friends. Don't worry if you cannot answer a question fully as you will discuss the solutions in the class.

9.0 Videos

Please watch this week's videos: V9.1, V9.2, V9.3, V9.4.

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

9.1

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

$$V(\boldsymbol{r}) = \begin{cases} 0, & 0 \leq r_i \leq L \\ \infty, & \text{otherwise} \end{cases} \tag{213}$$

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

9.1.1

Sketch the potential.

ANS: [cubic box]

9.1.2

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

ANS:

$$-\frac{\hbar^2}{2m}\left(\partial_x^2 + \partial_y^2 + \partial_z^2\right)\phi(\boldsymbol{r}) = E\phi(\boldsymbol{r})$$

inside the well/box, where ∂_x is for constant t, y, z.

9.1.3

Find the energy eigenvalues and normalised energy eigenstates.

ANS:

Let

$$\phi(\boldsymbol{r}) = X(x)\,Y(y)\,Z(z)$$
$$E = E_x + E_y + E_z$$

then we get three copies of the 1D case. For the x case,

$$X(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n_x \pi x}{L}\right)$$
$$E_x = \frac{\hbar^2 n_x^2 \pi^2}{2mL^2}.$$

Therefore

$$\phi(\boldsymbol{r}) = \left(\frac{2}{L}\right)^{3/2}\sin\left(\frac{n_x \pi x}{L}\right)\sin\left(\frac{n_y \pi y}{L}\right)\sin\left(\frac{n_z \pi z}{L}\right)$$

and

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

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.

ANS:

$2mL^2E/\hbar^2\pi^2$	n_x	n_y	n_z	degeneracy
3	1	1	1	1
6	1	1	2	3
9	1	2	2	3
11	1	1	3	3
12	2	2	2	1

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?

ANS:

for generic lengths (all relatively irrational), all levels are non-degenerate. If any two lengths are related by a rational number, however, degeneracies will return.

9.2 Angular momentum operators

9.2.1

State the commutation relation between any two angular momentum operators. Show that

$$\left[\hat{L}^2, \hat{L}_z\right] = 0. \tag{214}$$

ANS:

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

where ϵ_{ijk} is the Levi-Civita symbol and $\{i, j, k\} \in \{x, y, z\}$.

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

and so

$$\begin{aligned}
\left[\hat{L}^2, \hat{L}_z\right] &= \left[\hat{L}_x^2, \hat{L}_z\right] + \left[\hat{L}_y^2, \hat{L}_z\right] \\
&= \hat{L}_x\left[\hat{L}_x, \hat{L}_z\right] + \left[\hat{L}_x, \hat{L}_z\right]\hat{L}_x \\
&+ \hat{L}_y\left[\hat{L}_y, \hat{L}_z\right] + \left[\hat{L}_y, \hat{L}_z\right]\hat{L}_y \\
&= -i\hbar\hat{L}_x\hat{L}_y - i\hbar\hat{L}_y\hat{L}_x \\
&+ i\hbar\hat{L}_y\hat{L}_x + i\hbar\hat{L}_x\hat{L}_y \\
&= 0.
\end{aligned}$$

9.2.2

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

$$\hat{L}^2|l\rangle = \hbar^2 l\,(l+1)\,|l\rangle \tag{215}$$

$$\hat{L}_z|m\rangle = \hbar m|m\rangle \tag{216}$$

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

ANS:

since $\hat{L}_z$ and $\hat{L}^2$ commute they can have a joint set of eigenvectors (with different eigenvalues). Therefore it is reasonable to label the state by these two eigenvalues simultaneously, as they can be known simultaneously.

9.2.3

Defining

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y \tag{217}$$

show that

$$\left[\hat{L}_\pm, \hat{L}_z\right] = \mp\hbar\hat{L}_\pm. \tag{218}$$

ANS:

$$\begin{aligned}
\left[\hat{L}_\pm, \hat{L}_z\right] &= \left[\hat{L}_x \pm i\hat{L}_y, \hat{L}_z\right] \\
&= \left[\hat{L}_x, \hat{L}_z\right] \pm i\left[\hat{L}_y, \hat{L}_z\right] \\
&= -i\hbar\hat{L}_y \mp \hbar\hat{L}_x \\
&= \mp\hbar\left(\hat{L}_x \pm i\hat{L}_y\right).
\end{aligned}$$

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.

ANS:

$$\begin{aligned}
\hat{L}_z|m\rangle &= \hbar m|m\rangle \\
\hat{L}_\pm\hat{L}_z|m\rangle &= \hbar m\hat{L}_\pm|m\rangle \\
\left(\hat{L}_z\hat{L}_\pm + \left[\hat{L}_\pm, \hat{L}_z\right]\right)|m\rangle &= \hbar m\hat{L}_\pm|m\rangle \\
\left(\hat{L}_z\hat{L}_\pm \mp \hbar\hat{L}_\pm\right)|m\rangle &= \hbar m\hat{L}_\pm|m\rangle \\
\hat{L}_z\left(\hat{L}_\pm|m\rangle\right) &= \hbar\left(m \pm 1\right)\left(\hat{L}_\pm|m\rangle\right)
\end{aligned}$$

which defines the object in parentheses to be an eigenvalue of $\hat{L}_z$ with eigenvalue $\hbar\left(m \pm 1\right)$.

9.3

Consider the two-dimensional quantum harmonic oscillator defined by the Hamiltonian

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\omega^2\left(\hat{x}^2 + \hat{y}^2\right). \tag{219}$$

9.3.1

Explain why you might correctly expect that

$$[\hat{p}_x, \hat{p}_y] = [\hat{p}_x, \hat{y}] = [\hat{p}_y, \hat{x}] = [\hat{x}, \hat{y}] = 0.$$

ANS:

The operators are acting in perpendicular directions. Quantum mechanics is linear, so we might reasonably expect that what happens in the x direction has no bearing on what happens in y, as with usual linear superposition.

9.3.2

Show that the Hamiltonian can be rewritten

$$\hat{H} = \hbar\omega\left(\hat{n}_x + \hat{n}_y + \hat{\mathbb{I}}\right) \tag{220}$$

where

$$\hat{n}_x = \hat{a}_x^\dagger \hat{a}_x \tag{221}$$

and

$$\hat{a}_x = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}_x\right) \tag{222}$$

and similarly for y.

ANS:

Since x-directed and y-directed operators commute, this is just two copies of the 1D case added together! See PS8.

9.3.3

Explain why it is reasonable to label the energy eigenstates

$$\hat{H}|n_x, n_y\rangle = E_{n_x,n_y}|n_x, n_y\rangle. \tag{223}$$

State an expression for $|n_x, n_y\rangle$ in terms of the ground state $|0, 0\rangle$.

ANS:

as before, the operators commute, so we can find simultaneous eigenstates of both, and we can reasonably label such states by their eigenvalues under both operators.

$$|n_x, n_y\rangle = \frac{\left(\hat{a}_x^\dagger\right)^{n_x}}{\sqrt{n_x!}} \frac{\left(\hat{a}_y^\dagger\right)^{n_y}}{\sqrt{n_y!}} |0, 0\rangle.$$

9.3.4

Defining the operator

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \tag{224}$$

show that

$$\hat{L}_z = i\hbar \left(\hat{a}_y^\dagger \hat{a}_x - \hat{a}_x^\dagger \hat{a}_y\right). \tag{225}$$

Hence show that $\hat{L}_z$ commutes with neither $\hat{n}_x$ nor $\hat{n}_y$ individually, but does commute with $\hat{H}$. What does this tell us about the possible quantum numbers? Hence suggest an alternate labelling of the energy eigenstates.

ANS:

$$\begin{aligned}
\left[\hat{L}_z, \hat{n}_x\right] &= \left[i\hbar\left(\hat{a}_y^\dagger \hat{a}_x - \hat{a}_x^\dagger \hat{a}_y\right), \hat{a}_x^\dagger \hat{a}_x\right] \\
&= i\hbar\left[\hat{a}_y^\dagger \hat{a}_x, \hat{a}_x^\dagger \hat{a}_x\right] - i\hbar\left[\hat{a}_x^\dagger \hat{a}_y, \hat{a}_x^\dagger \hat{a}_x\right] \\
&= i\hbar\hat{a}_y^\dagger\left[\hat{a}_x, \hat{a}_x^\dagger \hat{a}_x\right] - i\hbar\hat{a}_y\left[\hat{a}_x^\dagger, \hat{a}_x^\dagger \hat{a}_x\right] \\
&= -i\hbar\hat{a}_y^\dagger \hat{a}_x^\dagger\left[\hat{a}_x, \hat{a}_x\right] - i\hbar\hat{a}_y^\dagger\left[\hat{a}_x^\dagger, \hat{a}_x\right]\hat{a}_x \\
&+ i\hbar\hat{a}_y \hat{a}_x^\dagger\left[\hat{a}_x, \hat{a}_x^\dagger\right] + i\hbar\hat{a}_y\left[\hat{a}_x^\dagger, \hat{a}_x^\dagger\right]\hat{a}_x \\
&= i\hbar\hat{a}_y^\dagger \hat{a}_x + i\hbar\hat{a}_y \hat{a}_x^\dagger.
\end{aligned}$$

A quick way to see that $\hat{L}_z$ commutes with $\hat{n}_x + \hat{n}_y$, and therefore commutes with $\hat{H}$, is to note that switching $x \leftrightarrow y$ switches $\hat{L}_z \to -\hat{L}_z$, so

$$\left[\hat{L}_z, \hat{n}_x\right] = -\left[\hat{L}_z, \hat{n}_y\right]$$

and so

$$\left[\hat{L}_z, \hat{n}_x + \hat{n}_y\right] = 0.$$

We already knew we can know n_x and n_y and E simultaneously, so that we can write energy eigenstates $|n_x, n_y\rangle$.
Now we also know that we can know $n \triangleq n_x + n_y$, the eigenstate of $\hat{L} + z$ (label it $\hbar m$), and E simultaneously, so we could equally well write the energy eigenstates $|n, m\rangle$.
But we *can't* know m, n_x, and n_y simultaneously, so the label $|n_x, n_y, m\rangle$ would be meaningless!

9.4

[#: you won't need to reproduce the derivation in an exam, but you should know where it comes from.] Starting from the definition of classical angular momentum in cartesian co-ordinates, derive the quantum operator $\hat{L}_z$ in spherical polar co-ordinates.
ANS:
Classically $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$. Quantum mechanically we promote observables to operators: $\hat{\boldsymbol{L}} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}$:

$$\hat{\boldsymbol{L}} = \begin{pmatrix} \hat{L}_x \\ \hat{L}_y \\ \hat{L}_z \end{pmatrix} = \begin{pmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{pmatrix} \times \begin{pmatrix} \hat{p}_x \\ \hat{p}_y \\ \hat{p}_z \end{pmatrix} = \begin{pmatrix} \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{x}\hat{p}_z - \hat{z}\hat{p}_x \\ \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \end{pmatrix}$$

and so, writing in the cartesian positon basis in which $\hat{x} = x$ and $\hat{p}_x = -i\hbar\partial_x$,

$$\hat{L}_z = -i\hbar \left(x\partial_y - y\partial_x \right).$$

Now convert to spherical polars:

$$\begin{aligned} x &= r\cos(\phi)\sin(\theta) \\ y &= r\sin(\phi)\sin(\theta) \\ z &= r\cos(\theta) \end{aligned}$$

$$\begin{aligned} r &= \sqrt{x^2 + y^2 + z^2} \\ \tan(\theta) &= \frac{\sqrt{x^2 + y^2}}{z} \\ \tan(\phi) &= y/x. \end{aligned}$$

chain rule:

$$\partial_x = (\partial_x r)\,\partial_r + (\partial_x \theta)\,\partial_\theta + (\partial_x \phi)\,\partial_\phi$$

etc. so we need 6 derivatives:

$$\partial_x r = x/r = \cos(\phi)\sin(\theta)$$
$$\partial_y r = y/r = \sin(\phi)\sin(\theta)$$

for the θ terms it's easiest to work implicitly:

$$\begin{aligned}\left(1+\tan^2(\theta)\right)\partial_x\theta &= \frac{x}{z\sqrt{x^2+y^2}} \\ \partial_x\theta &= \frac{z^2}{x^2+y^2}\frac{x}{z\sqrt{x^2+y^2}} \\ &= \frac{xz}{(x^2+y^2)^{3/2}} = \frac{\cos\phi\cos\theta}{r\sin^2\theta} \\ \partial_y\theta &= \frac{yz}{(x^2+y^2)^{3/2}} = \frac{\sin\phi\cos\theta}{r\sin^2\theta}.\end{aligned}$$

Finally

$$\begin{aligned}\tan(\phi) &= y/x \\ &\downarrow \partial_x \\ \left(1+\tan^2(\phi)\right)\partial_x\phi &= -y/x^2 \\ \left(1+y^2/x^2\right)\partial_x\phi &= -y/x^2 \\ \partial_x\phi &= \frac{-y}{x^2+y^2}\end{aligned}$$

giving

$$\begin{aligned}\partial_x\phi &= \frac{-y}{x^2+y^2} = -\frac{\sin\phi}{r\sin\theta} \\ \partial_y\phi &= \frac{x}{x^2+y^2} = \frac{\cos\phi}{r\sin\theta}\end{aligned}$$

Putting it together we get

$$\partial_x = \cos(\phi)\sin(\theta)\,\partial_r + \frac{\cos\phi\cos\theta}{r\sin^2\theta}\partial_\theta - \frac{\sin\phi}{r\sin\theta}\partial_\phi$$
$$\partial_y = \sin(\phi)\sin(\theta)\,\partial_r + \frac{\sin\phi\cos\theta}{r\sin^2\theta}\partial_\theta + \frac{\cos\phi}{r\sin\theta}\partial_\phi$$

and the final result simplifies massively:

$$\hat{L}_z = -i\hbar\,(x\partial_y - y\partial_x)$$
$$\hat{L}_z = -i\hbar\partial_\phi.$$

10 The Hydrogen Atom

Bring solutions along to the class at 10am on 7/12/20.

Questions marked # are beyond the syllabus. We may discuss them in the class if there is time.
Attempt all questions. Feel free to discuss with friends. Don't worry if you cannot answer a question fully as you will discuss the solutions in the class.

10.1 Spherically symmetric potentials

The TISE in spherical polar co-ordinates reads

$$\hat{H}\psi(\boldsymbol{r},t) = E\psi(\boldsymbol{r},t) \tag{226}$$

where

$$\hat{H} = -\frac{\hbar^2}{2\mu r^2}\partial_r\left(r^2\partial_r\right) + \frac{1}{2\mu r^2}\hat{L}^2 + V(\boldsymbol{r}) \tag{227}$$

and

$$\hat{L}^2 = -\hbar^2\left(\frac{1}{\sin(\theta)}\partial_\theta\left(\sin(\theta)\partial_\theta\right) + \frac{1}{\sin^2(\theta)}\partial_\phi^2\right). \tag{228}$$

The symbol μ here is used in place of m for the mass of the particle. In the hydrogen atom μ will be the reduced mass.

Explain why, if the potential is symmetric such that $V(\boldsymbol{r}) = V(r)$ where $\boldsymbol{r} = (r,\theta,\phi)$, the TISE is separable using the ansatz

$$\psi(\boldsymbol{r},t) = T(t)R(r)Y(\theta,\phi). \tag{229}$$

Carry out the separation, and, defining the separation constant $\hbar^2k^2$, write down the radial and angular equations.

ANS:

in the case that $V = V(r)$ the Hamiltonian is just a sum of operators acting on either r or (θ,ϕ). This is a sufficient condition for separability. In this case,

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

$$\downarrow$$

$$\frac{1}{R}\hbar^2\partial_r\left(r^2\partial_r\right)R + \frac{2mr^2}{R}(E-V)R = \frac{1}{Y}\hat{L}^2Y \triangleq \hbar^2k^2$$

and so we have 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

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

10.2 Angular equation

Explain why the angular equation is itself separable. Using the ansatz

$$Y\left(\theta, \phi\right) = P\left(\cos\left(\theta\right)\right) F\left(\phi\right) \tag{230}$$

and separation constant m^2 write down the azimuthal equation for θ and the polar equation for ϕ. Show that both are now ordinary differential equations (ODEs).

ANS:

$$\begin{aligned} \hat{L}^2 Y &= \hbar^2 k^2 Y \\ -\sin\left(\theta\right) \partial_\theta \left(\sin\left(\theta\right) \partial_\theta\right) Y - \sin^2\left(\theta\right) k^2 Y &= \partial_\phi^2 Y \end{aligned}$$

so it's again a sum of terms acting solely on either θ or ϕ.

$$\frac{1}{P} \sin\left(\theta\right) \partial_\theta \left(\sin\left(\theta\right) \partial_\theta\right) P + \sin^2\left(\theta\right) k^2 = -\frac{1}{F} \partial_\phi^2 F \triangleq m^2$$

giving the polar equation

$$\frac{\mathrm{d}^2 F}{\mathrm{d}\phi^2} = -m^2 F$$

and azimuthal equation

$$\sin\left(\theta\right) \frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\left(\theta\right) \frac{\mathrm{d}}{\mathrm{d}\theta}\right) P + \sin^2\left(\theta\right) k^2 P = m^2 P.$$

Both are ODEs as they only contain a single variable.

10.2.1 Polar equation

Show that the solutions to the polar equation take the form

$$F(\phi) = A\exp(\pm im\phi) \tag{231}$$

with A a complex constant. Thinking about the meaning of ϕ in the spherical polar co-ordinate system, explain why you might expect m to be restricted to integers. Show that $F_m(\phi)$ are eigenstates of $\hat{L}_z$. What physical observable does the operator $\hat{L}_z$ correspond to? Therefore explain the physical meaning of m being integer.

ANS:

the stated form solves the polar equation. Since $\phi + 2\pi$ is equivalent to ϕ in the polar system, we expect $F(\phi + 2\pi) \equiv F(\phi)$ and so $\exp(\pm 2\pi im) \equiv 1$, requiring m to be an integer. There is actually some subtlety here, as strictly it's only $|F|^2$ which is observable and must remain single-valued, but the more complex argument leads to the same result.

$\hat{L}_z$ is the operator associated with the z-projection of angular momentum.

$$\hat{L}_z = -i\hbar\partial_\phi$$

(see PS9) and so

$$\hat{L}_z F_m = \pm\hbar m F_m.$$

Therefore m being an integer implies the z-projection of angular momentum is quantized.

10.2.2 Azimuthal equation

By making the change of variables

$$x = \cos(\theta) \tag{232}$$

show that the azimuthal equation can be rewritten as the *associated Legendre equation*:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\left(1 - x^2\right)\frac{\mathrm{d}}{\mathrm{d}x}\right)P(x) + \left(l(l+1) - \frac{m^2}{1 - x^2}\right)P(x) = 0 \tag{233}$$

giving an equation for l. The solutions $P_l^m(x)$ are called the associated Legendre polynomials, and are valid for $l \geq 0$ integer and $|m| \leq l$ integer. Find the un-normalised solutions $P_0^0(x)$ and $P_1^0(x)$.

ANS:

$$\sin(\theta)\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin(\theta)\frac{\mathrm{d}}{\mathrm{d}\theta}\right)P(x) + \sin^2(\theta)k^2P(x) = m^2P(x)$$

and note that

$$\frac{\mathrm{d}x}{\mathrm{d}\theta}\frac{\mathrm{d}}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}\theta}$$

so

$$-\sin(\theta)\frac{\mathrm{d}}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}\theta}$$

giving

$$\left(1-x^2\right)\frac{\mathrm{d}}{\mathrm{d}x}\left(\left(1-x^2\right)\frac{\mathrm{d}}{\mathrm{d}x}\right)P(x) + \left(1-x^2\right)k^2 P(x) = m^2 P(x)$$
$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\left(1-x^2\right)\frac{\mathrm{d}}{\mathrm{d}x}\right)P(x) + \left(k^2 - \frac{m^2}{1-x^2}\right)P(x) = 0.$$

Therefore the equation is returned if $k^2 = l(l+1)$. For $m = l = 0$

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\left(1-x^2\right)\frac{\mathrm{d}}{\mathrm{d}x}\right)P(x) = 0$$

which is solved by a constant. For $m = 0$, $l = 1$

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\left(1-x^2\right)\frac{\mathrm{d}}{\mathrm{d}x}\right)P(x) + 2P(x) = 0$$
$$-2xP'(x) + \left(1-x^2\right)P'' + 2P(x) = 0$$

which is solved by Ax.

10.3 Radial equation

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

$$\hbar^2\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}}{\mathrm{d}r}\right)R_l(r) + 2mr^2(E-V)R_l(r) = \hbar^2 l(l+1)R_l(r). \tag{234}$$

ANS:

We established that $k^2 = l(l+1)$, hence the form of the equation, and that l is an integer quantum number which can label the solutions. Since l appears in this equation, R must carry it as a quantum number. This will in general be alongside the principal quantum number n labelling the energy.

10.4 The hydrogen atom

10.4.1

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

$$\left(-\frac{\hbar^2}{2\mu r^2}\partial_r\left(r^2\partial_r\right)+\frac{\hbar^2 l\left(l+1\right)}{2\mu r^2}-\frac{e^2}{4\pi\epsilon_0 r}\right)\varphi_{n,l,m}\left(\boldsymbol{r}\right)=E_n\varphi_{n,l,m}\left(\boldsymbol{r}\right). \tag{235}$$

ANS:

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

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

The labels n, l, and m are all good quantum numbers.

10.4.2

Using the ansatz

$$\varphi_{n,l,m}\left(\boldsymbol{r}\right)=\frac{\chi_{n,l}\left(r\right)}{r}Y_l^m\left(\theta,\phi\right) \tag{236}$$

show that the radial equation can be rewritten

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2\chi_{n,l}\left(r\right)}{\mathrm{d}r^2}-\frac{e^2}{4\pi\epsilon_0 r}\chi_{n,l}\left(r\right)+\frac{\hbar^2 l\left(l+1\right)}{2mr^2}\chi_{n,l}\left(r\right)=E_n\chi_{n,l}\left(r\right). \tag{237}$$

ANS:

The Y term factors out, leaving

$$\begin{aligned}
-\frac{\hbar^2}{2\mu}\partial_r\left(r^2\partial_r\right)\left(\chi/r\right)+\frac{\hbar^2 l\left(l+1\right)}{2\mu r}\chi-\frac{e^2}{4\pi\epsilon_0}\chi&=E_n r\chi\\
-\frac{\hbar^2}{2\mu}\partial_r\left(r\chi'-\chi\right)+\frac{\hbar^2 l\left(l+1\right)}{2\mu r}\chi-\frac{e^2}{4\pi\epsilon_0}\chi&=E_n r\chi\\
-\frac{\hbar^2}{2\mu}\left(\chi'+r\chi''-\chi'\right)+\frac{\hbar^2 l\left(l+1\right)}{2\mu r}\chi-\frac{e^2}{4\pi\epsilon_0}\chi&=E_n r\chi\\
-\frac{\hbar^2}{2\mu}\chi''+\frac{\hbar^2 l\left(l+1\right)}{2\mu r^2}\chi-\frac{e^2}{4\pi\epsilon_0 r}\chi&=E_n\chi
\end{aligned}$$

as required.

10.4.3

Defining the Bohr radius

$$a_0 \triangleq \frac{4\pi\epsilon_0\hbar^2}{\mu e^2} \tag{238}$$

the dimensionless radial co-ordinate

$$\rho \triangleq \frac{r}{a_0} \tag{239}$$

the dimensionless energy variable

$$\lambda^2 \triangleq -\frac{2\mu E a_0^2}{\hbar^2} \tag{240}$$

and the rescaled function

$$\Xi(\rho) \triangleq \chi(r) \tag{241}$$

show that the radial equation can be rewritten

$$\Xi''(\rho) - \frac{l(l+1)}{\rho^2}\Xi(\rho) + \frac{2}{\rho}\Xi(\rho) = \lambda^2\Xi(\rho) \tag{242}$$

where the primes now indicate derivatives with respect to ρ rather than r.

ANS:

Just substitute it all in.

10.4.4

Show that in the limit $\rho \gg 1$ the solution takes the form

$$\Xi(\rho) = A\exp(-\lambda\rho) \tag{243}$$

and in the limit $\rho \ll 1$ it takes the form

$$\Xi(\rho) = B\rho^{l+1}. \tag{244}$$

ANS:

In the limit $\rho \gg 1$ the $1/\rho$ and $1/\rho^2$ terms tend to zero, leaving

$$\Xi''(\rho) = \lambda^2\Xi(\rho)$$

with solution

$$\Xi(\rho) = A\exp(\pm\lambda\rho)$$

for real λ. The growing solution would not be normalizable (the domain is $0 \leq \rho \leq \infty$). In the limit $\rho \ll 1$ the terms to survive are those with the most negative powers of ρ, i.e.

$$\Xi''(\rho) = \frac{l(l+1)}{\rho^2}\Xi(\rho)$$

which is solved by the stated form.

10.4.5 #

These limiting forms suggest the following ansatz:

$$\Xi(\rho) = \rho^{l+1}\exp(-\lambda\rho)\,\alpha(2\lambda\rho). \tag{245}$$

Defining

$$y = 2\lambda\rho \tag{246}$$

Show that this leads to Laguerre's equation:

$$y\alpha''(y) + \alpha'(y)(2(l+1) - y) - \left(l + 1 - \frac{1}{y}\right)\alpha(y) = 0 \tag{247}$$

where primes now indicate derivatives with respect to y. The solutions are the Laguerre polynomials $L^{2l+1}_{n-l-1}(y)$ with $n > 0$ an integer, where the eigenvalues are

$$E_n = \frac{-\hbar^2}{2\mu a_0^2 n^2}. \tag{248}$$

ANS:

$$\Xi''(\rho) - \frac{l(l+1)}{\rho^2}\Xi(\rho) + \frac{2}{\rho}\Xi(\rho) = \lambda^2\Xi(\rho)$$
$$\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\left(\frac{l+1}{\rho} - \lambda + 2\lambda\frac{\alpha'(2\lambda\rho)}{\alpha(2\lambda\rho)}\right)\Xi\right) - \frac{l(l+1)}{\rho^2}\Xi + \frac{2}{\rho}\Xi = \lambda^2\Xi$$
$$\left(\frac{l+1}{\rho} - \lambda + 2\lambda\frac{\alpha'(2\lambda\rho)}{\alpha(2\lambda\rho)}\right)^2 - \frac{l+1}{\rho^2} + 4\lambda^2\frac{\alpha''(2\lambda\rho)}{\alpha(2\lambda\rho)} - 4\lambda^2\left(\frac{\alpha'}{\alpha}\right)^2 - \frac{l(l+1)}{\rho^2} + \frac{2}{\rho} = \lambda^2$$
$$(l+1-\lambda\rho)^2\alpha + 4\lambda\rho(l+1-\lambda\rho)\alpha' - (l+1)\alpha + 4\lambda^2\rho^2\alpha''(2\lambda\rho) - l(l+1)\alpha + 2\rho\alpha = \lambda^2\rho^2\alpha$$
$$[1/\lambda - (l+1)]\alpha + 2(l+1-y/2)\alpha' + y\alpha'' = 0$$

and so (phew!)

$$y\alpha'' + \alpha'(2(l+1) - y) - (l+1-1/\lambda)\alpha = 0.$$

10.4.6

Put everything together to find the (un-normalised) energy eigenfunctions of the hydrogen atom $\psi_{n,l,m}(\boldsymbol{r}, t)$.

ANS:

$$\psi_{n,l,m}(\boldsymbol{r}) \propto r^l \exp\left(-\sqrt{-2\mu E_n}r/\hbar\right) L_{n-l-1}^{2l+1}\left(2\sqrt{-2\mu E_n}r/\hbar\right) P_l^m(\cos(\theta)) \exp(\pm im\phi) \exp(-iE_n t/\hbar).$$

10.5 The Bohr model

10.5.1

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.

10.5.2

Assuming (incorrectly) that the electron orbits the nucleus classically, equate the centripetal force to the electrostatic force to obtain an expression for the velocity in terms of the radius (and other quantities). Hence derive Bohr's formula for the radius of possible orbits:

$$r_n = \frac{4\pi\epsilon_0 n^2 \hbar^2}{e^2 m_e} \tag{249}$$

and find the Bohr radius r_1 (conventionally denoted a_0).

ANS:

$$L = m_e v r = n\hbar, \ \ n \in \mathbb{Z} > 0.$$

Equating the centripetal force and electrostatic force gives

$$mr\omega^2 = \frac{e^2}{4\pi\epsilon_0 r^2}$$

where the signs are the same as the force is directed from the electron to the nucleus in both cases. Using $v = r\omega$ gives

$$v = \frac{e}{\sqrt{4\pi\epsilon_0 mr}}$$

and substituting into the Bohr quantization condition gives

$$n\hbar = e\sqrt{\frac{mr}{4\pi\epsilon_0}}$$

and so

$$r_n = \frac{4\pi\epsilon_0 n^2\hbar^2}{me^2}.$$

Then

$$a_0 = r_1 = \frac{4\pi\epsilon_0\hbar^2}{me^2} = \frac{4\pi\cdot 8.9\times 10^{-12}\,\mathrm{Fm}^{-1}\left(1.055\times 10^{-34}\,\mathrm{Js}\right)^2}{9.11\times 10^{-31}\,\mathrm{kg}\cdot\left(1.609\times 10^{-19}\,\mathrm{C}\right)^2} = \frac{4\pi\cdot 8.9\cdot 1.1^2}{9.1\cdot 1.6^2}\times 10^{-11}\,\mathrm{m}$$

$$a_0 = 5.3\times 10^{-11}\,\mathrm{m}.$$

10.5.3

Using the same model, show that the energy levels of the atom are:

$$E_n = \frac{m_e e^4}{2\left(4\pi\epsilon_0\right)^2\hbar^2 n^2}. \tag{250}$$

Use this formula to calculate the ionization energy of hydrogen.

ANS:

$$\begin{aligned} E = \frac{1}{2}mv^2 &= \frac{m}{2}\left(\frac{e}{\sqrt{4\pi\epsilon_0 mr}}\right)^2 \\ &= \frac{e^2}{2\cdot 4\pi\epsilon_0 r} \\ &= \frac{e^2}{2\cdot 4\pi\epsilon_0}\frac{me^2}{4\pi\epsilon_0 n^2\hbar^2} \end{aligned}$$

as required. The ionization energy is the energy to excite the electron from state $n=1$ to $n=\infty$ (unbound), so

$$E_{\text{ionization}} = \frac{m_e e^4}{\left(4\pi\epsilon_0\right)^2 2\hbar^2} = 13.6\,\mathrm{eV}.$$

10.5.4

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

ANS:

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

$$r_n^{\text{positronium}} = 2r_n^H$$
$$E_n^{\text{positronium}} = \frac{1}{2}E_n^H.$$

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.

10.5.5

A 656.3 nm photon is detected from a hydrogen atom. What is the principal quantum number of the electron in the atom immediately after this detection?

ANS:

The energy of the photon must be the difference in energy of the two levels transitioned between:

$$f = c/\lambda = 4.6 \times 10^{14}\,\text{Hz}$$
$$E = hf = 3.1 \times 10^{-19}\,\text{J}$$
$$= 1.9\,\text{eV}.$$

Therefore

$$1.9\,\text{eV} = 13.6\,\text{eV}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$
$$0.14 = \frac{1}{n_1^2} - \frac{1}{n_2^2}.$$

Try the first few cases:

n_1	n_2	$n_1^{-2} - n_2^{-2}$
1	2	0.75
2	3	0.14

where we abandoned $n_1 = 1$ after the first attempt as all subsequent n_2 would give a larger value, and we needed a smaller value. So the transition must have been from $n_2 = 3$ to $n_1 = 2$ (the photon was emitted, so energy was lost), and the answer is 2.